

10/694,845

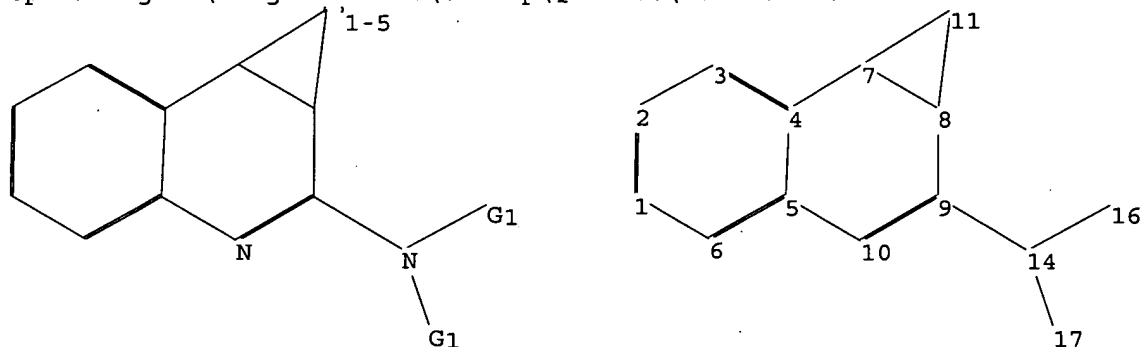
* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:37:17 ON 08 SEP 2005

=> file reg

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Uploading C:\Program Files\Stnexp\Queries\10694845.str



chain nodes :

14 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

9-14 14-16 14-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-11 8-9 8-11 9-10

exact/norm bonds :

4-7 5-10 7-8 7-11 8-9 8-11 9-10 9-14 14-16 14-17

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:C,H,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 14:CLASS 16:CLASS 17:CLASS

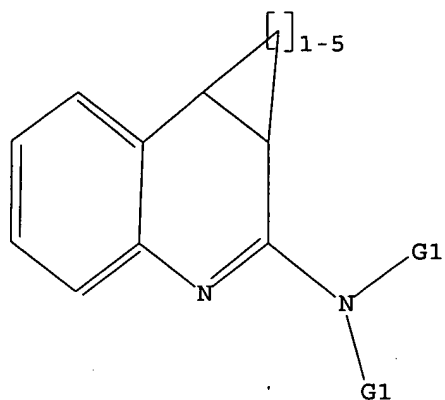
L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

10/694,845



G1 C,H,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

L3 666 SEA SSS FUL L1

=> file ca

=> s l3

L4 151 L3

=> s l4 an py<1999

MISSING OPERATOR L4 AN

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l4 and py<1999

18655783 PY<1999

L5 90 L4 AND PY<1999

=> s l5 and (pharm? or drug?)

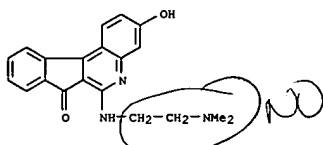
522458 PHARM?

730437 DRUG?

L6 12 L5 AND (PHARM? OR DRUG?)

=> d ibib abs fhitstr 1-12

L6 ANSWER 1 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 129:183768 CA
 TITLE: TAS-103: antineoplastic topoisomerase I and II inhibitor
 AUTHOR(S): Hoshi, A.; Castaner, J.
 CORPORATE SOURCE: Tokyo, 125, Japan
 SOURCE: Drugs of the Future (1998), 23(5), 513-515
 CODEN: DRFUD4; ISSN: 0377-8282
 PUBLISHER: Prous Science
 DOCUMENT TYPE: Journal; General Review
 LANGUAGE: English
 AB A brief review with 24 refs., describing synthesis, pharmacol. actions, mechanism of action, toxicity, and clin. studies of the indeno[2,1-c]-quinolin-7-one derivative TAS-103, an antineoplastic topoisomerase I and II inhibitor.
 IT 174634-08-3P, 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-
 RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (TAS-103, antineoplastic topoisomerase I and II inhibitor)
 RN 174634-08-3 CA
 CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)

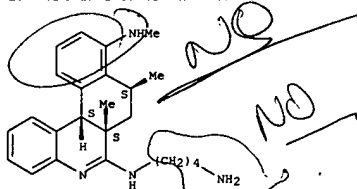


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 2 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 128:265841 CA
 TITLE: Inhibition of tumor growth and polyamine uptake by tetracyclic amidines bearing a putrescine moiety
 AUTHOR(S): Mens, T.; Tomasi, S.; Elfier-Lima, V. L.; Uriac, P.; Huet, J.; Catros-Quemener, V.
 CORPORATE SOURCE: Groupe de Recherche en Therapeutique Anticancereuse, UPRES-A CNRS 6027, Faculte de Medecine de Rennes, Rennes, 35043, Fr.
 SOURCE: Anticancer Research (1997), 17(6D), 4327-4332
 CODEN: ANTRD4; ISSN: 0250-7005
 PUBLISHER: Anticancer Research
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Tetracyclic amidines (tetrahydroquino[4,3-b][1]benzazepine (I) and tetrahydrobenzo[k]naphthyridine (II)) bearing a putrescine moiety possess significant DNA-binding affinity. The authors report here that these compds. and their a and b isomers inhibit tumor cell growth and putrescine uptake in 3LL carcinoma cells in vitro. Moreover, I reduced by 50% the accumulation of putrescine in intestinal brush border membrane vesicles. In CHO-MG, a cell line deficient for the specific polyamine uptake system, the cytotoxicity of these compds. was significantly reduced compared to the CHO wild cell line. The IC50 for CHO-MG was significantly higher than for CHO, demonstrating that the polyamine transport system increased the efficacy of these compds. The efficacy of I and II might therefore be related to their ability to interact with DNA as well as their structural analogy with polyamines. Moreover, the authors clearly show that DFMO enhances the efficacy of these tetracyclic amidines in vivo. Potential mechanisms include: (a) lower intracellular polyamine levels reduces polyamine DNA-stabilizing functions, increasing accessibility for DNA-binding drugs; (b) DFMO enhances the polyamine uptake system in tumor cells, increasing the entry of tetracyclic amidines bearing a putrescine moiety as well as their accessibility to final DNA-binding sites. The fact that natural polyamine uptake is reduced by the same compds. constitutes an additive mechanism for antitumoral efficiency.
 IT 205697-81-0
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (inhibition of tumor growth and polyamine uptake by tetracyclic amidines bearing a putrescine moiety)
 RN 205697-81-0 CA
 CN Benzo[k]phenanthridine-6,9-diamine, N6-(4-aminobutyl)-6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-, (6aa,8a,12ba)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

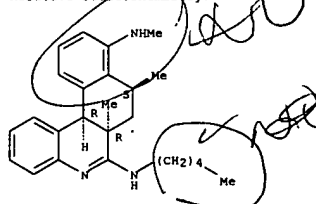
L6 ANSWER 2 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 3 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 127:257203 CA
 TITLE: Depletion of polyamines potentiates the antitumor effect of tetracyclic amidines bearing a putrescine moiety
 AUTHOR(S): Tomasi, S.; Elfier-Lima, V. L.; Le Roch, M.; Corbel, J. C.; Renault, J.; Uriac, P.; Mens, T.; Catros-Quemener, V.; Moulinoux, J. P.
 CORPORATE SOURCE: UPRES de Pharmacochimie de Molecules de Synthese et de
 SOURCE: Substances Naturelles, Faculte de Pharmacie, Rennes, 35043, Fr.
 Pharmaceutical Sciences (1997), 3(5/6), 241-247
 CODEN: PHSCFB; ISSN: 1356-6881
 PUBLISHER: Royal Pharmaceutical Society of Great Britain
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB D,L-2-(difluoromethyl)ornithine (DFMO), a potent inactivator of putrescine biosynthesis that depletes spermidine levels in cells, is known to enhance cytotoxicity of DNA-binding drugs. A significant in-vitro cytotoxicity and DNA-binding affinity found for amidines containing both heterocyclic and polyamine moieties prompted the authors to evaluate their in-vivo activity on Lewis lung carcinoma (3LL). When administered alone to tumor bearing mice, neither DFMO nor the tetracyclic amidines were effective. However, their combined administration with DFMO inhibited tumor growth significantly.
 IT 196296-15-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (depletion of polyamines with DFMO potentiates antitumor effect of tetracyclic amidines bearing a putrescine moiety)
 RN 196296-15-8 CA
 CN Benzo[k]phenanthridine-6,9-diamine, 6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-N6-pentyl-, (6aa,8b,12ba)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

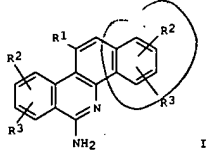
10/694,845

L6 ANSWER 3 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 4 OF 12 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 126:330558 CA
TITLE: Preparation of aminobenzophenanthridine derivatives
INVENTOR(S): Clement, Bernd
PATENT ASSIGNEE(S): Germany
SOURCE: Ger. Offen., 5 pp.
CODEN: GWKXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19538088	A1	19970417	DE 1995-19538088	19951013
CA 2232609	AA	19970424	CA 1996-2232609	19961011
WO 9714683	A2	19970424	WO 1996-DE1958	19961011
WO 9714683	A3	20010913		
W: AU, BG, BR, CA, CN, CZ, HU, IL, JP, KP, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9715895	A1	19970507	AU 1997-15895	19961011
AU 707092	B2	19990701		
EP 873315	A1	19981028	EP 1996-945501	19961011
EP 873315	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1204321	A	19990106	CN 1996-197596	19961011
JP 11515001	T2	19991221	JP 1996-515415	19961011
BR 9610971	A	19991228	BR 1996-10971	19961011
IL 123692	A1	20001121	IL 1996-123692	19961011
RU 2180333	C2	20020310	RU 1998-108615	19961011
AT 238284	E	20030515	AT 1996-945501	19961011
CZ 291821	B6	20030618	CZ 1998-1074	19961011
NO 9801655	A	19980611	NO 1998-1655	19980408
NO 313328	B1	20020916		
US 6030981	A	20000229	US 1998-51606	19980413
PRIORITY APPLN. INFO.:			DE 1995-19538088	A 19951013
			WO 1996-DE1958	W 19961011
OTHER SOURCE(S):		MARPAT 126:330558		
GI				

L6 ANSWER 4 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)

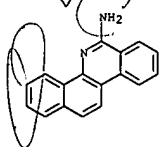


AB Aminobenzophenanthridine derivs. I [R1 = H, aryl, heteroaryl; R2, R3 = alkoxy, alkenyloxy, halogen, NO2] and their 11,12-dihydro derivs. were prepared for use as pharmaceuticals (no data). Thus, 2-MeC6H4CN was dimerized with CH2O in presence of Me3COK in DMPU to give 16% 6-amino-11,12-dihydrobenzo[c]phenanthridine hydrochloride which was treated with DDQ in dioxane to give 44% 6-aminobenzo[c]phenanthridine perchlorate.

IT 189577-92-2P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminobenzophenanthridine derivs.)
RN 189577-92-2 CA
CN Benzo[c]phenanthridin-6-amine, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 189577-91-1
CMF C17 H12 N2



CM 2

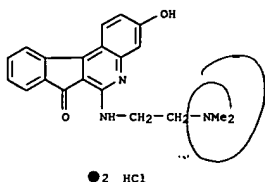
CRN 7601-90-3
CMF C1 H O4



L6 ANSWER 5 OF 12 CA COPYRIGHT 2005 ACS on STN

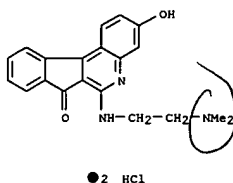
ACCESSION NUMBER: 126:258391 CA
TITLE: Simultaneous determination of a novel anticancer drug, TAS-103, and its N-demethylated metabolite in monkey plasma by high-performance liquid chromatography using solid-phase extraction
AUTHOR(S): Azuma, Ryotaro; Urakawa, Akira
CORPORATE SOURCE: Pharmacokinetics Research Laboratory, Taiho Pharmaceutical Co., Ltd., 224-2, Ebisuno, Hiraishi, Kawauchi-cho, Tokushima, Japan
SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1997), 691(1), 179-185
CODEN: JCBBEF; ISSN: 0378-4347
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A simple and rapid method for the anal. of a novel anticancer drug, TAS-103, and its metabolite demethyl-TAS-103 in monkey plasma has been developed. This method is based on high-performance liquid chromatog. with visible detection at 460 nm after solid-phase extraction with a Sep-Pak Vac PS-2 cartridge. The extraction recoveries of each compound, including the internal standard TAS-1-018, were from 88 to 102. The quantitation limit of each compound was 5.0 ng/mL in 0.5 mL of plasma. The coeffs. of variation for each compound ranged from 0.9 to 4.9, and relative errors for each compound ranged from -3.8 to 4.6. Both compds. in monkey plasma were stable at -80°C for 39 days and the exts. were stable at ambient temperature for 24 h. This method has been demonstrated to be useful for the pharmacokinetic study of TAS-103 in monkey plasma after i.v. administration.
IT 174634-09-4, TAS 103
RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)
(determination of TAS-103 and its N-demethylated metabolite in plasma by HPLC using solid-phase extraction)
RN 174634-09-4 CA
CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[(2-(dimethylamino)ethyl)amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)



L6 ANSWER 6 OF 12 CA COPYRIGHT 2005 ACS on STN

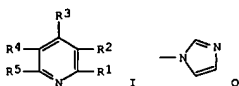
126:238248 CA
 TITLE: Theory and actual attempts to establish an effective cancer chemotherapy
 AUTHOR(S): Fujimoto, Shuichi
 CORPORATE SOURCE: Division of Chemotherapy, Chiba Cancer Center, Research Institute, Japan
 SOURCE: Gan to Kagaku Ryoho (1997), 24(4), 501-510
 CODEN: GTRDX; ISSN: 0385-0684
 PUBLISHER: Gan to Kagaku Ryohosha
 DOCUMENT TYPE: Journal: General Review
 LANGUAGE: Japanese
 AB A review with 9 refs. To establish an effective cancer chemotherapy, theor. analyses of chemoresistance factors in recurrent patients and possible approaches to curative chemotherapy were under-taken. Multidrug resistance of tumor cells in recurrent patients may hamper the development of new antitumor agents. Thus, we developed a new screening method (FACS method) which employs fresh clin. specimens. By this method, TAS-103 was found to be far more effective than 10 standard drugs and to be one of the most effective drugs among 20 or more new antitumor agents under study. Development of several effective drugs, such as TAS-103, might lead to a curative cancer chemotherapy.
 IT 174634-09-4, TAS 103
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (theory and actual attempts to establish an effective cancer chemotherapy)
 RN 174634-09-4 CA
 CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 12 CA COPYRIGHT 2005 ACS on STN
 116:235628 CA
 TITLE: Preparation of pyridines and related aza heterocycle derivatives as antihypertensives and antiarrhythmics
 INVENTOR(S): Tomcufcik, Andrew Stephen; Meyer, Walter Edward; Marsico, Joseph William
 PATENT ASSIGNEE(S): American Cyanamid Co., USA
 SOURCE: Eur. Pat. Appl., 48 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 446604	A2	19910918	EP 1991-101496	19910205
EP 446604	A3	19920219		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
JP 04217958	A2	19920807	JP 1991-73934	19910313
CA 2038317	AA	19910917	CA 1991-2038317	19910314
AU 9173525	A1	19910919	AU 1991-73525	19910315
AU 640208	B2	19930819		
PRIORITY APPLN. INFO.:			US 1990-494387	A 19900316

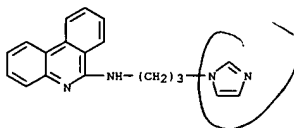
OTHER SOURCE(S): MARPAT 116:235628
 GI



AB The title compds. [I: R1 = H, halo, NR6ZR7; R2 = H, NO2, cyano; R1R2 = CH3CH2CH2; R3 = H, C1-3 alkyl, Ph, NR6ZR7, R2R3 = R1R2; R4 = H, NO2, cyano, C1-3 alkyl, COMe, CONH2; R3R4 = R1R2; R5 = H, halo, C1-3 alkyl, C6H4CF3-3, C6H4F-3, C6H2(OMe)3-3,4,5, pyridyl; R4R5 = R1R2, CH3C(OMe)CH2CH, NNPN, SCH2CH, etc.; R6 = H, COMe; R7 = pyridyl, imidazol; Z = (CH2)n; n = 1-5; with a proviso] and their pharmaceutically acceptable salts were prepared, e.g., by amination of chloropyridines with R7Z-amines. Thus, refluxing for 16 h a mixture of 31.7 g 2-chloro-3-nitropyridine and 50 g Q(CH2)3NH2 in 500 mL EtOH in the presence of EtN(CHMe2)2 gave 43.7 g title compound I [R1 = NH(CH2)3Q, R2 = NO2, R3 = R4 = R5 = H (II)] which at 1 + 10⁻⁵ M gave 80% inhibition of TXB2. II in rats at 100 mg/kg (by gavage) reduced blood pressure to 98 from 160 mmHg, and in mice at 10 mg/kg i.v. in a CaCl2- and KCl-induced arrhythmia test gave survival rate 3/6 and 4/6, resp. Approx. 69 I were prepared

L6 ANSWER 7 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)

140692-33-7P
 IT 140692-33-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as antihypertensive and antiarrhythmic)
 RN 140692-33-7 CA
 CN 6-Phenanthridinamine, N-[3-(1H-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

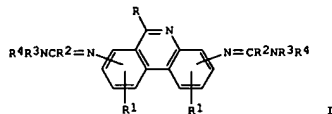


L6 ANSWER 8 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 103:160409 CA
 TITLE: Chemotherapeutic bisamidine derivatives of

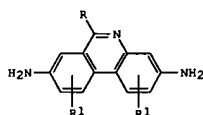
phenanthridines and their pharmaceutically acceptable salts
 PATENT ASSIGNEE(S): Hoechst Pharmaceuticals Ltd., India
 SOURCE: Indian, 26 pp.
 CODEN: INXXAP
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 153442	A	19840714	IN 1981-BO344	19811222
PRIORITY APPLN. INFO.:			IN 1981-BO344	19811222

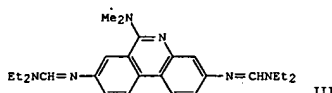
GI



I



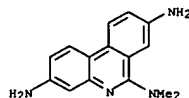
II



III

AB Phenanthridines I [R = H, halo, alkoxy, NH₂, monoalkylamino, dialkylamino,
 N heterocyclyl optionally containing O, S, N; R₁ = H, alkyl, alkoxy,
 halo,
 NO₂, NH₂; R₂ = H, (un)substituted alkyl; R₃, R₄ = H, alkyl; C(R₂)R₃N =

L6 ANSWER 8 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
 heterocyclyl; NR₃R₄ = heterocyclyl] were prepd. by treating
 diaminoanthridines II with R₂CONR₃R₄ and POCl₃. Thus,
 3,8-diamino-6-dimethylaminophenanthridine was added to a mixt. of Et₂NCHO
 and POCl₃ to give 71% phenanthridine III. I are useful as amebicides and
 protozoacides (no data).
 IT 93494-47-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (condensation of, with diethylformamide)
 RN 93494-47-4 CA
 CN 3,6,8-Phenanthridinetriamine, N₆,N₆-dimethyl- (9CI) (CA INDEX NAME)



L6 ANSWER 9 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 81:13559 CA
 TITLE: Benzazine derivatives
 INVENTOR(S): Rodway, Ronald E.; Cookson, Ronald F.
 PATENT ASSIGNEE(S): Aspro-Nicholas Ltd.
 SOURCE: S. African, 138 pp.
 CODEN: SFXKAB
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

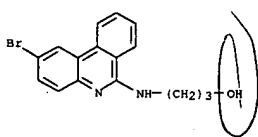
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 7201118	A	19731031	ZA 1972-1118	19720221
PRIORITY APPLN. INFO.:			ZA 1972-1118	A 19720221

GI For diagram(s), see printed CA Issue.

AB Benzazine compds. I-VII [X = CH₂CH₂, CH = CH, (CH₂)₃, R, R₁ = H, Ph,
 substituted Ph, NO₂, halo] with analgesic, antiinflammatory,
 antibacterial, antiviral and cardiovascular activity were prepared
 Thus, a mixture of phenyl phthalazone and ethylene-diamine monotosylate was
 heated at 240° for 20 hr, extracted with hot dilute HCl and then basified with
 NaOH to give II (X = CH₂CH₂, R = Ph).

IT 38052-92-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 38052-92-5 CA
 CN 1-Propanol, 3-[(2-bromo-6-phenanthridinyl)amino]- (9CI) (CA INDEX NAME)



L6 ANSWER 10 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 43:8385 CA
 ORIGINAL REFERENCE NO.: 43:1778g-1,1779a-e
 TITLE: New syntheses of heterocyclic compounds. IX.
 Tetrahydrophenanthridines
 AUTHOR(S): Hollingsworth, B. L.; Petrow, V.
 SOURCE: Journal of the Chemical Society, Abstracts (1948) 1537-41
 CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 43:8385

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 41, 9671. Work on the relationship between structure and
 analgetic activity has been extended by the preparation of some 9-amino-
 and

tetrahydro-9-aminophenanthridines (I, R = NH₂) by direct amination of the
 corresponding bases (the pharmacol. data will be published by
 Thorp). Cyclohexanone (50 g.), 9 g. (NCHO)₃, and 11 g. Et₂NH.HCl, heated
 until the Mannich base is formed, treated with 9.3 g. PhNH₂, 12.8 g.
 PhNH₂.HCl, and 13 g. SnCl₄.5H₂O and refluxed 16 h., give 45%
 5,6,7,8-tetrahydrophenanthridine (Ia) (I, R = H), m. 63° (C.A. 31,
 7061.9); omission of SnCl₄ reduced the yield to 15% and of PhNH₂.HCl to
 less than 5%. o-MeC₆H₄NH₂ gives 40% of the 1-Me derivative of Ia and
 p-MeC₆H₄NH₂ gives 50% of the 3-Me derivative m-MeC₆H₄NH₂ gives 15% of

the 2(or
 4)-Me derivative, b₂₀ 210° [picrate, yellow, m. 226°
 (decomposition)]. 5-Methyl-1-(diethylaminomethyl)-2-cyclohexanone and

PhNH₂ give 12% of the 7-Me derivative of Ia. 3,5-Me₂C₆H₃NH₂ gives 20% of the
 1,3-di-Me derivative of Ia and 2,5-Me₂C₆H₃NH₂ gives 20% of the
 1,4-isomer.

o-MeC₆H₄NH₂ gives 25% of the 1-MeO derivative of Ia, yellow, m.
 106° [picrate, mustard-yellow, m. 214° (decomposition)];
 p-MeC₆H₄NH₂ gives 50% of the 3-MeO isomer. p-O₂NC₆H₄NH₂ yields 50% of

the 3-NO₂ derivative of Ia, m. 172-3° [picrate, m. 203° (decomposition)].
 p-ClC₆H₄NH₂ gives 30% of the 3-Cl derivative of Ia. p-PhC₆H₄NH₂ yields
 40% of

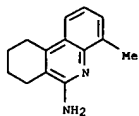
the 3-Ph derivative of Ia, m. 122-3° [picrate, yellow, m. 235°
 (decomposition)]. 1-(1-Naphthyliminomethyl)-2-cyclohexanone (II) (50
 g.) and

400 mL. anhydrous HCO₂H, refluxed 20 h., give 60% 5,6,7,8-tetrahydro-1,2-
 benzophenanthridine and the 2-naphthyl isomer of II gives 75% of the
 3,4-isomer. 5-Aminoacenaphthene and formylcyclohexanone give
 1-(5-acenaphthyliminomethyl)-2-cyclohexanone, orange-yellow, m.
 137-8°; this yields 50% 1,2,3,4-tetrahydro-11-aza-6,7-acenchrysene
 (III), cream, m. 134-5° [picrate, yellow, m. 252-3°
 (decomposition)]. Ia (5 g.), 25 g. PhNH₂, and 6 g. NaNH₂, heated 5 h.

at 170°, give 4 g. of the 9-NH₂ derivative (IV), m. 165°; acetate,
 prepared in excess hot AcOH, m. 212-13°. IV (5 g.) in 300 mL. dilute
 HCl, treated with 4 g. NaNO₂ in 40 mL. ice-cold H₂O and heated 1 h. on

the water bath, gives 4 g. 5,6,7,8-tetrahydrophenanthridone, m. 272°.
 9-Amino-1-methyl-5,6,7,8-tetrahydrophenanthridine, m. 121-2°, 45%;
 3-Me isomer, m. 169-70°, 90% (acetate m. 204-5°); 1,3-di-Me
 derivative, m. 136-7°, 60%. 9-Amino-5,6,7,8-tetrahydro-3,4-
 benzophenanthridine, m. 241-2°, 80%. The 1-Me derivative of Ia (10 g.)
 and 10 g. Se, heated 5 h. at 300°, give 85% 1-methylphenanthridine,

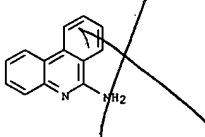
L6 ANSWER 10 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
 m. 95^o; 7 g., 25 mL. PhNH₂, and 8 g. NaNH₂, heated 4 h. at 160^o, give 501 of the 9-NH₂ deriv., m. 116-17^o.
 9-Amino-3-methylphenanthridine, m. 170-1^o, 601; the 1,3-di-Me compd. m. 142-3^o, 551.
 IT 855623-05-1, Phenanthridine, 6-amino-7,8,9,10-tetrahydro-4-methyl- (preparation of)
 RN 855623-05-1 CA
 CN Phenanthridine, 6-amino-7,8,9,10-tetrahydro-4-methyl- (5CI) (CA INDEX NAME)



L6 ANSWER 11 OF 12 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 33:22099 CA
 ORIGINAL REFERENCE NO.: 33:3173a-d
 TITLE: Picrylamino compounds; diazelines
 INVENTOR(S): Morgan, Gilbert T.; Stewart, Jessie
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

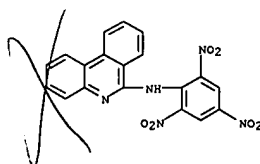
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 496258		19381128	GB	

AB Picrylamino, compds. are prepared by condensing picryl chloride (I) or an alkyl derivative thereof, e. g., methyl- and dimethyl-picryl chlorides, with a compound containing a tertiary cyclic N atom and an adjacent amino group, e. g., 2-aminopyridine (II), 2-aminoquinoline, 1-aminoisoquinoline, 9-aminophenanthridine and their homologs. By cautious heating, preferably in the presence of PhOH, dimethylaniline, etc., ring closure takes place with formation of dinitro-1,3-diazelines, from which 1,3-diazelines may be obtained by reduction and elimination of the amino groups formed. The products are useful as intermediates for the manufacture of dyes and drugs. Among examples, (1) I is heated in C₆H₆ solution with II to give N-picryl-2-aminopyridine; when PhMe is used as solvent, ring closure takes place with formation of 1,2-pyrido-7,9-dinitro-4,5-benzo-1,3-diazaline, (2) by heating the diazaline of (1) with an aqueous solution of Na polysulfide, 1,2-pyrido-7,9- or -9,7-nitroamino-4,5-benzo-1,3-diazaline is produced; when H is used as reducing agent under an initial pressure of 5 atmospheric and in the presence of Pt oxide, 1,2-pyrido-7,9-diamino-4,5-benzo-1,3-diazaline (III) is produced while at H pressures maintained at 8-10 atmospheric tetrahydro-III results.
 IT 832-68-8, Phenanthridine, 6-amino- (ring closure of derivs. of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



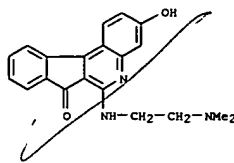
L6 ANSWER 12 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
 ACCESSION NUMBER: 33:3973 CA
 ORIGINAL REFERENCE NO.: 33:5941,595a-i,596a-d
 TITLE: Pyrido(1',2',1,2)benzimidazoles and allied compounds (cyclic 1,3-diazelines)
 AUTHOR(S): Morgan, Gilbert T.; Stewart, Jessie
 SOURCE: Journal of the Chemical Society, Abstracts (1938) 1292-305
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB The α-NH₂ derivs. of pyridine, quinoline and isoquinoline readily obtainable from these bases by the NaNH₂ condensation are favorable starting materials in the preparation of substances having a pyridinic or quinolinic structure likely to be of interest as either color intermediates or therapeutic agents. 5-Amino-2,2'-dipyridylamine (I), m. 91^o, results from catalytic reduction of the 5-NO₂ derivative in absolute EtOH at 50^o. 2-Aminopyridine (II) and 2,4-(O₂N)C₆H₃Cl, heated at 120^o for 2 hrs., give N,2',4'-dinitrophenyl-2-aminopyridine (III), golden needles, m. 156-7^o; I gives N,2',4'-dinitrophenyl-5-amino-2,2'-dipyridylamine (IV), red, m. 198^o; these 2 NO₂ derivs. possess tinctorial properties toward acetate rayon similar to the Dispersol yellows. Catalytic reduction of III gives the di-NH₂ derivative, m. 150^o; the di-NH₂ derivative from IV m. 187^o. II and picryl chloride, refluxed in C₆H₆ for 1 hr., give N,2',4',6'-trinitrophenyl-2-aminopyridine (V), m. 135^o; I gives N,2',4',6'-trinitrophenyl-5-amino-2,2'-dipyridylamine, ruby-red, m. 224^o. V forms a N-Me derivative, bright red, m. 243^o. V may be represented in 2 tautomeric forms on the supposition that the H atom of the picramido group migrates to the adjacent N atom of the C₅H₅N ring; in 1 case, on loss of HNO₂, a dinitro-α-carboline would result, in the other a di-NO₂ derivative of a new hydroaromatic base (VI), designated pyrido(1',2',1,2)benzimidazole (numbering as in VII) or 1,2-pyrido-4,5-benzo-1,3-diazaline (numbering as in VIII). Refluxing V in PhNH₂ for 2-2.5 hrs. gives the 4,6-di-NO₂ derivative (IX) of VI, bright yellow, m. above 300^o; PhNH₂2. In PhNO₂, PhOH in PhNO₂ or PhOH alone also give IX; V also gives IX on heating at 135^o until frothing ceases and then at 200-20^o; IX also results when V is prepared in PhMe in place of C₆H₆. Catalytic reduction of IX gives the 4,6-di-NH₂ derivative (X), yellow, m. 204-5^o, while Na₂S in 50% aqueous Me₂CO gives the 4,6(or 6,4)-nitroamino derivative of VI, dark red, m. above 280^o. Removal of the NH₂ group by reduction of the diazo compound with 50% EtOH gives the 4(or 6)-NO₂ derivative of VI, bright yellow, m. 260-2^o; catalytic reduction gives the 4(or 6)-NH₂ derivative (XI), yellow, m. 229-30^o. Removal of the NH₂ group from XI or the 2 NH₂ groups from X gives VI, m. 178-9^o; it has an aniseed-like odor, while the isomeric α-carboline (XII) is odorless; unlike XII, VI does not exhibit pronounced blue fluorescence in neutral solvents nor does it develop on reduction the characteristic deep blue color with p-Me₂NC₆H₄CHO. Catalytic reduction of VI in EtOH at 50^o (PtO₂ at 10-8 atmospheric) gives the 3',4',5',6'-tetrahydro derivative of X, m. 201-2^o; a higher H₂ pressure or a higher temperature did not cause further reduction; through the diazo reaction this yields the 3',4',5',6'-tetrahydro derivative

L6 ANSWER 12 OF 12 CA COPYRIGHT 2005 ACS on STN (Continued)
 of VI, m. 107^o. The diazo compd. from VIII with NaN₃ gives 4,6-bis(triazopyrido(1',2',1,2)benzimidazole, C₁₁H₆N₈, decomp. 167-70^o; the 3',4',5',6'-tetrahydro deriv. m. 132^o. 2-Amino-3-methylpyridine and picryl chloride in C₆H₆ give N-picryl-2-amino-3-methylpyridine, yellow, m. 142-3^o; PhOH in xylene gives 4,6-dinitro-3'-methylpyrido(1',2',1,2)benzimidazole (XIII), yellow, m. 256-60^o; catalytic reduction of XIII gives the di-NH₂ deriv., yellow, m. about 130^o; Na₂S and S in dil. aq. Me₂CO reduce XIII to the 4,6(or 6,4)-nitroamino deriv., red, m. 269-70^o; removal of the NH₂ group gives the 4(or 6)-NO₂ deriv., yellow, m. 260-2^o and reduced catalytically to the 4(or 6)-NH₂ deriv., m. 185-7^o; removal of this NH₂ group gives 3'-methylpyrido(1',2',1,2)benzimidazole, m. 162^o. 2-Aminoquinoline yields a picryl deriv., yellow, m. above 280^o; heating with an equal wt. of PhOH in xylene gives 4,6-dinitroquinolo(1',2',1,2)benzimidazole, yellow, m. above 300^o; the 4,6-di-NH₂ deriv., yellow, m. 273-4^o, results in 75% yield on catalytic reduction in abs. EtOH at an initial pressure of 31 atm. The 4,6(or 6,4)-nitroamino deriv., brick-red, m. above 300^o; the 4(or 6)-NO₂ deriv., yellow, m. 242-3^o; this gives the yellow-green 4(or 6)-NH₂ deriv., m. 223^o. Quinolo(1',2',1,2)benzimidazole, m. 102^o, results from either the mono- or di-NH₂ deriv. 1-Aminoisoquinoline yields a red picryl deriv., m. 156^o; PhOH in xylene gives 4,6-dinitroisoquinolo(2',1',1,2)benzimidazole, golden needles, m. above 280^o; the 4,6-di-NH₂ deriv. m. 249-50^o; reduction of the diazo compd. with abs. EtOH gives isoquinolo(2',1',1,2)-benzimidazole, m. 129^o which becomes a pale pink-buff on exposure to light and air. 9-Aminophenanthridine reacts with picryl chloride only in boiling xylene and the resulting picryl deriv. is contaminated with XIV; the pure deep yellow infusible deriv. could be obtained by using small quantities of the reactants. Boiling the mixt. with PhNH₂2 gives 4,6-dinitrophenanthrido(10',9',1,2)benzimidazole (XIV), deep yellow, m. above 280^o; 4,6-di-NH₂ deriv., yellow, the reduction being carried out at 80-90^o with an initial H₂ pressure of 31 atm.; removal of the NH₂ groups gives phenanthrido(10',9',1,2)benzimidazole, m. 153-4^o.
 IT 861002-25-7, Phenanthridine, 6-(2,4,6-trinitroanilino)- (preparation of)
 RN 861002-25-7 CA
 CN Phenanthridine, 6-(2,4,6-trinitroanilino)- (4CI) (CA INDEX NAME)



L8 ANSWER 1 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 128:43507 CA
 TITLE: Antitumor activity of a novel quinoline derivative, TAS-103, with inhibitory effects on topoisomerases I and II
 AUTHOR(S): Utsugi, Teruhiro; Aoyagi, Kumio; Asao, Tetsuji; Okazaki, Shinji; Aoyagi, Yoshimi; Sano, Masaki; Wierzbna, Konstanty; Yamada, Yuji
 CORPORATE SOURCE: Hanno Research Center, Taiho Pharmaceutical Co., Ltd.,
 SOURCE: Hanno, 357, Japan
 Japanese Journal of Cancer Research (1997), 88(10), 992-1002
 CODEN: JJCREP; ISSN: 0910-5050
 PUBLISHER: Japanese Cancer Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A novel quinoline derivative, TAS-103 (6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-7H-indeno[2,1-c]quinolin-7-one dihydrochloride), was developed as an anticancer agent targeting topoisomerases (topo) I and II, with marked efficacy in solid tumors. TAS-103 inhibited topo I and II (IC50: 2 μ M, 6.5 μ M) at a concentration similar to or lower than those of previous agents, and had a strong cytotoxic effect on P388 and KB cells (IC50: 0.0011 μ M, 0.0096 μ M). TAS-103 stabilized top I and II-DNA complex to that induced by etoposide (VP-16) but a smaller amount of topo I-DNA complex than that produced by camptothecin (CPT). In the in vivo study, intermittent i.v. administration was markedly effective against s.c.-implanted murine tumors. Furthermore, TAS-103 had marked efficacy against various lung metastatic tumors, and a broad antitumor spectrum in human tumor xenografts (derived from lung, colon, stomach, breast, and pancreatic cancer). The efficacy of TAS-103 was generally greater than that of irinotecan (CP-11), VP-16, or cis-diaminedichloroplatinum (CDDP).
 IT 174634-09-4, TAS-103
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study);
 USES (Uses)
 (antitumor activity of TAS-103 and inhibitory effects on topoisomerases I and II)
 RN 174634-09-4 CA
 CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



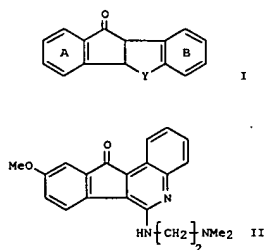
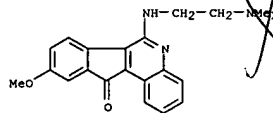
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L8 ANSWER 2 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 127:81361 CA
 TITLE: Preparation of indenoquinoline derivatives and analogs
 INVENTOR(S): as antitumor agents
 Asao, Tetsuji; Okazaki, Shinji; Wakita, Sukeji; Utsugi, Teruhiro; Yamada, Yuji
 PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
 CODEN: JKXKAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09143166	A2	19970603	JP 1995-299420	19951117
JP 3643916	B2	20050427	JP 1995-299420	19951117

 PRIORITY APPLN. INFO.:
 OTHER SOURCE(S): MARPAT 127:81361
 GI

L8 ANSWER 2 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 RN 191801-82-8 CA
 CN 11H-Indeno[1,2-c]quinolin-11-one, 6-[[2-(dimethylamino)ethyl]amino]-9-methoxy-, dihydrochloride (9CI) (CA INDEX NAME)

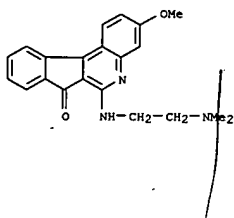


AB The title compds. I [ring A, B = benzene ring which may have substituents such as halo, alkoxy, etc.; Y = R1C=N, etc.; R1 = NR3R4, etc.; R3, R4 = H, Ph, etc.] are prepared. The title compound II.2HCl at 225 mg/kg/day for 2 days gave 35% increase in the survival time of mice with transplanted P388 leukemic cells.
 IT 191801-82-8P
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of indenoquinoline derivs. and analogs as antitumor

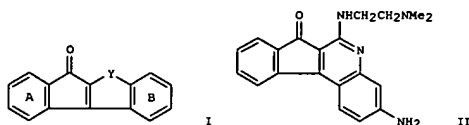
L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN
 124:232268 CA
 TITLE: Preparation and formulation of indenoquinolines as antitumor agents
 INVENTOR(S): Okazaki, Shinji; Asao, Tetsuji; Wakida, Motoji; Ishida, Keisuke; Washinosu, Masato; Utsugi, Teruhiro; Yamada, Yuji
 PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 146 pp.
 CODEN: PIXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9532187	A1	19951130	WO 1995-JP944	19950518
W: AU, CA, CN, FI, HU, JP, KR, NO, NZ, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 440562	B	20010616	TW 1995-84104882	19950517
AU 9524542	A1	19951218	AU 1995-24542	19950518
AU 685631	B2	19980122		
ZA 9504077	A	19960119	ZA 1995-4077	19950518
EP 713870	A1	19960529	EP 1995-918733	19950518
EP 713870	B1	20010718		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1130903	A	19960911	CN 1995-190639	19950518
CN 1131216	B	20031217		
HU 75651	A2	19970528	HU 1996-130	19950518
HU 218308	B	20000728		
JP 2840796	B2	19981224	JP 1995-530192	19950518
RU 2124017	C1	19981227	RU 1996-105034	19950518
CA 2167382	C	19990831	CA 1995-2167382	19950518
IL 113778	A1	19990922	IL 1995-113778	19950518
AT 203236	E	20010815	AT 1995-918733	19950518
ES 2158109	T3	20010901	ES 1995-918733	19950518
PT 713870	T	20011130	PT 1995-918733	19950518
FI 9600280	A	19960318	FI 1996-280	19960119
FI 111721	B1	20030915		
NO 9600239	A	19960318	NO 1996-239	19960119
NO 305555	B1	19990621		
US 5733918	A	19980331	US 1996-578542	19960119
US 5710162	A	19980120	US 1996-713224	19960912

L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

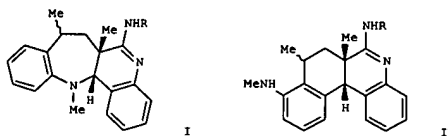


L8 ANSWER 3 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 US 6028079 A 20000222 US 1997-909934 19970812
 GR 3036795 T3 20020131 GR 2001-401657 20011004
 PRIORITY APPLN. INFO.: JP 1994-107190 A 19940520
 WO 1995-JP944 W 19950518
 US 1996-578542 A3 19960119
 OTHER SOURCE(S): MARPAT 124:232268
 GI



AB The title compds. I (ring A represents an optionally substituted benzene or naphthalene ring, or a benzene ring having an lower alkylenedioxy group; ring B represents a benzene ring which may be substituted or has a lower alkylenedioxy group; Y represents N:CR or CR(N); R represents NR1R2, OR3 or an optionally substituted nitrogenous heterocyclic group;
 R1 and R2 are the same or different from each other and each represents hydrogen, Ph, an optionally substituted nitrogenous heterocyclic group, or a lower alkyl group which may be substituted by at least one substituent selected from the group consisting of optionally substituted amino, lower alkoxy, Ph, a nitrogenous heterocyclic group, an amine oxide group substituted by lower alkyl, and hydroxy; and R3 represents lower alkyl which may be substituted by substituted amino, provided the case where R represents an optionally substituted nitrogenous heterocyclic group and rings A and B represent each an unsubstituted benzene ring, is excluded) are prepared. The title compound II.3HCl (preparation given) in vitro showed IC50 of 1.1 x 10⁻² µg/mL against p388 mouse leukemic cells.
 IT 174634-05-09
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of indenoquinolines as antitumor agents)
 RN 174634-05-0 CA
 CN 7H-Indeno[2,1-c]quinolin-7-one, 6-[(2-(dimethylamino)ethyl)amino]-3-methoxy- (9CI) (CA INDEX NAME)

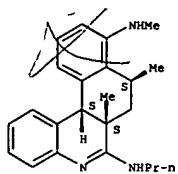
L8 ANSWER 4 OF 77 CA COPYRIGHT 2005 ACS on STN
 124:202063 CA
 ACCESSION NUMBER: 124:202063 CA
 TITLE: Relationship between cytotoxicity and DNA-binding affinity of amidine derivatives of tetrahydroquino[4,3-b][1]benzazepines and tetrahydrobenzo[k]naphthyridines
 AUTHOR(S): Elfer-Lima, V. L.; Uriac, P.; Huet, J.; Jenkins, T. C.; Thurston, D. E.
 CORPORATE SOURCE: Lab. Chim. Pharmaceutique, Fac. Pharmacie, Rennes, 35043, Fr.
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1995), 5(24), 3003-6
 CODEN: BMCLES; ISSN: 0960-894X
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Amidines I and II [R = Pr, (CH2)3OH, (CH2)3NH2, (CH2)4NH2] have been synthesized. All the compds. showed weak but significant DNA-binding affinity which correlated with in vitro cytotoxicity across two cell lines.
 IT 173960-71-9P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process) (preparation, DNA binding, and cytotoxicity of aminoquinobenzazepines and aminobenzonaphthyridines)
 RN 173960-71-9 CA
 CN Benzo[k]phenanthridine-6,9-diamine, 6a,7,8,12b-tetrahydro-N9,6a,8-trimethyl-N6-propyl-, dihydrochloride, (6a,8a,12ba)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 4 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



● 2 HCl

L8 ANSWER 5 OF 77 CA COPYRIGHT 2005 ACS on STN

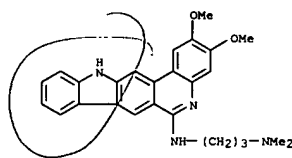
ACCESSION NUMBER: 123:32984 CA
 TITLE: A Versatile Construction of the 8H-Quino[4,3-b]carbazole Ring System as a Potential DNA Binder
 AUTHOR(S): Mohanakrishnan, Arasambattu K.; Srinivasan, Panayencheri C.
 CORPORATE SOURCE: Department of Organic Chemistry, University of Madras,
 Madras, 600 025, India
 SOURCE: Journal of Organic Chemistry (1995), 60(7), 1939-46
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A short synthesis of quino[4,3-b]- and quino[3,4-b]carbazoles is reported.
 The key step involves the preparation of suitable 2,3-divinylindoles by consecutive Wittig reactions. The thermal electrocyclic reaction of the divinylindole, with concomitant dehydrogenation in the presence of Pd-C, gave the (nitroaryl)carbazole, which, on reductive cyclization, led to the

the quinocarbazole. Cleavage of the phenylsulfonyl group, followed by phosphorus oxychloride treatment and subsequent displacement of the chlorine with 3-(dimethylamino)propylamine, gave the title compds. in 25-30% overall yield.

IT 164261-69-29
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of quinocarbazole ring systems)

RN 164261-69-2 CA
 CN 1,3-Propanediamine, N'-(2,3-dimethoxy-5,12-dihydro-12H-indolo[3,2-j]phenanthridin-6-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 122:187249 CA
 TITLE: Preparation of 2-phenanthridinylcarbenes as antibacterial agents
 INVENTOR(S): Dininno, Frank P.; Greenlee, Mark L.; Rano, Thomas A.;
 Lee, Wendy
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: PCT Int. Appl., 115 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: 1

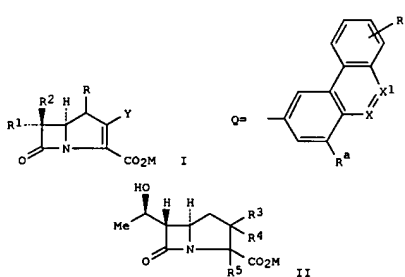
PATENT NO. KIND DATE APPLICATION NO. DATE
 WO 9417066 A1 19940804 WO 1994-US85 19940103

W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CH, GA, GN, ML, MR, NE, SN, TD, TG
 US 5336674 A 19940809 US 1993-9626 19930127

CA 2154276 AA 19940804 CA 1994-2154276 19940103
 AU 9459902 A1 19940815 AU 1994-59902 19940103
 EP 682666 A1 19951122 EP 1994-906014 19940103
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
 JP 08505874 T2 19960625 JP 1994-517039 19940103
 PRIORITY APPLN. INFO.: US 1993-9626 A 19930127
 WO 1994-US85 W 19940103

OTHER SOURCE(S): MARPAT 122:187249
 GI

L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

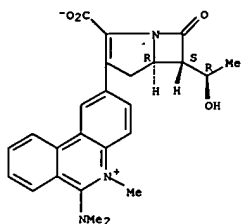


AB Title compds. [I: M = H, alkali metal, neg. charge, etc.; R = H, Me; R1, R2 = H, Me, Et, CH2OH, MeCH(OH), etc.; Y = phenanthridinyl group Q; 1 of Ra = H and the others = H, CF3, halo, (un)substituted alkoxy; 1 of X, X1 = N-Rdm and the other = CRc; Rc = H, (un)substituted alkyl (oxy), NH2, etc.; Rd = H, NH2, O-, alkyl, etc.; m = 0 or 1] were prepared as antibacterial agents (no data). Thus, oxopenamcarboxylate II (M = CH2C6H4(NO2)-4, R3R4 = O, R5 = H) was condensed with Me3SnO CF3SO3- (Ra = H, X = N-Me, X1 = CH) and the product hydrogenolized to give II (M = neg. charge, R3 = Q, R4R5 = bond, Ra = H, X = N-Me, X1 = CH).

IT 161546-79-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of phenanthridinylcarbenes as antibacterial agents)
 RN 161546-79-8 CA
 CN Phenanthridinium, 2-[2-carboxy-6-(1-hydroxyethyl)-7-oxo-1-azabicyclo[3.2.0]hept-2-en-3-yl]-6-(dimethylamino)-5-methyl-, inner salt, [5R-[5a,6a(R')]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 6 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN

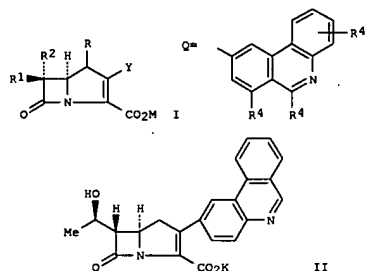
122:187248 CA
 TITLE: 2-(phenanthridinyl)carbapenem antibacterial agents
 INVENTOR(S): Dinunno, Frank P.; Greenlee, Mark L.; Rano, Thomas A.;

PATENT ASSIGNEE(S): Lee, Wendy
 Merck and Co., Inc., USA
 SOURCE: U.S., 28 pp.
 CODEN: USXXAM

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5328904	A	19940712	US 1993-9622	19930127
CA 2154275	AA	19940804	CA 1994-2154275	19940103
WO 9417065	A1	19940804	WO 1994-US62	19940103
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CH, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9461207	A1	19940815	AU 1994-61207	19940103
EP 682667	A1	19951122	EP 1994-907775	19940103
JP 08505873	T2	19960625	JP 1994-517034	19940103
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
PRIORITY APPLN. INFO.: US 1993-9622 A 19930127				
WO 1994-US62 W 19940103				
OTHER SOURCE(S): MARPAT 122:187248				
GI				

L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 7 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

AB The title compds. [I; M = H, carboxyl-protecting group, alkali metal; R = H, Me; R1, R2 = H, Me, Et, Me2CH, HOCH2, etc.; Y = Q, (un)substituted phenanthridinyl, etc.; R4 = H, CF3, halogen, Cl-4 alkoxy], useful as antibiotics (no data), are prepared. Thus, carbapenem II was prepared from

2-bromophenanthridine in 3 steps.

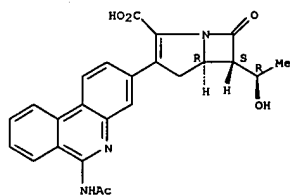
IT 161667-42-1

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (preparation of 2-(phenanthridinyl)carbapenem antibacterial agents)

RN 161667-42-1 CA

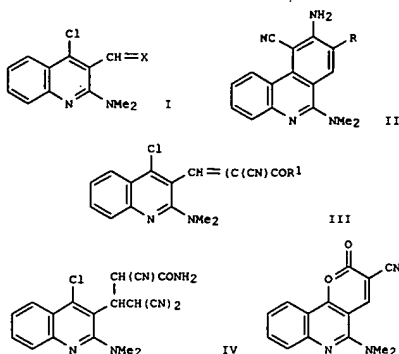
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[6-(acetylamino)-3-phenanthridinyl]-6-(1-hydroxyethyl)-7-oxo-, monosodium salt, [5R-[5a,6a(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



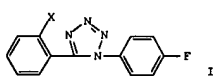
● Na

L8 ANSWER 8 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 121:300738 CA
 TITLE: Reactions of 2-(dimethylamino)-3-formyl-4-chloroquinoline with cyanoacetic acid derivatives
 AUTHOR(S): Nesterova, I. N.; Alekseyeva, L. M.; Granik, V. G.
 CORPORATE SOURCE: VNIIRFI, Moscow, Russia
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1993), 27(1), 71-5
 CODEN: KHFZAN; ISSN: 0023-1134
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

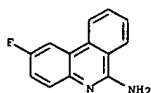


AB The conversion of quinoline derivative I (X = O) to compds. such as I (X = C(CN)2), II (R = CN, CO2Et), III (R1 = NH2, OEt), IV, and V is reported.
 IT 159112-49-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 159112-49-9 CA
 CN 8,10-Phenanthridinedicarbonitrile, 9-amino-6-(dimethylamino)- (9CI) (CA INDEX NAME)

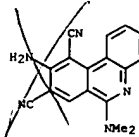
L8 ANSWER 9 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 120:323392 CA
 TITLE: Cyclizations. Part 1. Electrochemical and photochemical reactions of 1-(4-fluorophenyl)-5-(2-halogenophenyl)tetrazoles
 AUTHOR(S): Donnelly, Shileen; Grimshaw, James; Trocha-Grimshaw, Jadwiga
 CORPORATE SOURCE: Sch. Chem., Queen's Univ., Belfast, BT9 5AG, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (14), 1557-62
 CODEN: JCPRB; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



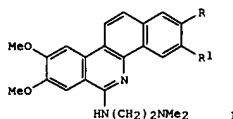
AB Electrochem. reduction of the title compds. I (R = Cl, Br, I) leads to cleavage of the carbon-halogen bond to leave a Ph radical. Competition then follows between intramol. radical substitution giving 7-fluorotetrazolo[1,5-f]phenanthridine and further reduction of the radical, then protonation, giving 1-(4-fluorophenyl)-5-phenyltetrazole. Substitution predominates but reduction and protonation becomes a more competing reaction when X = Br, I. Photochem. reaction of I confirms competition between C-X bond cleavage to give 7-fluorotetrazolo[1,5-f]phenanthridine and loss of nitrogen followed by cyclization to give 2-halophenyl-5-fluorobenzimidazole. C-X bond cleavage predominates and becomes the only reaction when the X = I. The fluorine substituent permits determination of product yields by 19F NMR spectroscopy.
 IT 153386-16-4P
 RL: PREP (Preparation) (formation in electrochem. reduction of fluorotetrazolophenanthridine)
 RN 153386-16-4 CA
 CN 6-Phenanthridinamine, 2-fluoro- (9CI) (CA INDEX NAME)



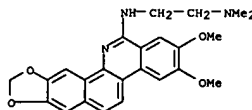
L8 ANSWER 8 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



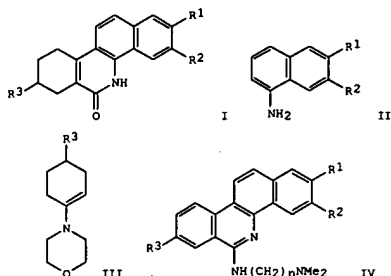
L8 ANSWER 10 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 120:270904 CA
 TITLE: A formal new access to the benzo[c]phenanthridine alkaloids, synthesis of nitidine and O-methyl fagarone analog
 AUTHOR(S): Janin, Yves L.; Bisagni, Emile
 CORPORATE SOURCE: Sect. Biol., Inst. Curie, Orsay, 91405, Fr.
 SOURCE: Tetrahedron (1993), 49(45), 10305-16
 CODEN: TETRA; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:270904
 GI



AB Previously unreported 2-aryl-1-naphthylamines were obtained in good yields from 2-aryl-1-tetralone oximes by using the Semmler-Wolf reaction but omitting the acetic anhydride usually present in the reaction mixture. From these amines, through the thermal cyclization of their corresponding Et carbonates, a new access to the benzo[c]phenanthridin-6(SH)-ones was found. Preparation of water-soluble nitidine and O-Me fagarone analogs bearing an alkylamino side chain on the C-6 position I (RR1 = OCH2O; R = R1 = MeO) was achieved from these compds.
 IT 154283-53-1P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 154283-53-1 CA
 CN 1,2-Ethanediamine, N'-(2,3-dimethoxy[1,3]benzodioxolo[5,6-c]phenanthridin-13-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)

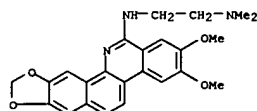


L8 ANSWER 11 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 120:270049 CA
 TITLE: Synthesis and evaluation of new 6-amino-substituted benzo[c]phenanthridine derivatives
 AUTHOR(S): Janin, Yves L.; Croisy, Alain; Riou, Jean Francois; Bisagni, Emile
 CORPORATE SOURCE: Sect. Biol. Inst. Curie, Inst. Curie, Orsay, F-91405, Fr.
 SOURCE: Journal of Medicinal Chemistry (1993), 36(23), 3686-92
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:270049
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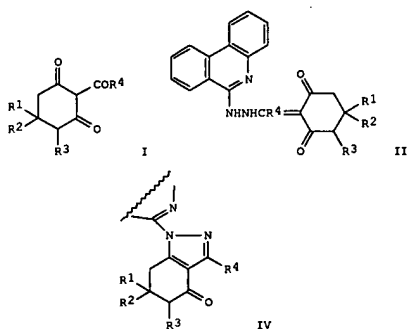
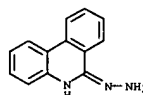
AB 7,8,9,10-Tetrahydrobenzo[c]phenanthridin-6(5H)-ones I (R1-R3 = H; R1 = R3 = OMe, R2 = H; R1 = R3 = H, R2 = OMe; R1 = OMe, R2 = R3 = H; R1 = OCHMe2, R2 = H, R3 = OMe) were prepared by using a one-pot procedure which includes the preparation of various 6- and 7-alkoxy-1-naphthyl isocyanates from 1-naphthylamines II and triphosgene, followed by addition of 1-morpholino-1-cyclohexenes III, and cyclization of the resulting amides upon heating in the presence of hydrogen chloride. Subsequent aromatization, chlorination, and substitution with [(dimethylamino)alkyl]amines, followed by a demethylation or a selective desisopropylation, allowed synthesis of benzo[c]phenanthridine derivs. IV (R1 = H, OMe, OCHMe2, OH; R2 = H, OMe, OH; R3 = H, OMe, OH; n = 2, 3) bearing a [(dimethylamino)alkyl]amino side chain at their 6-position. These compds. were devised to further study the structure-activity

L8 ANSWER 11 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 relationships in the benzo[c]phenanthridine family of antitumor alkaloids led by fagaronine and nitidine. Topoisomerases I and II cleavable complex assay and evaluation of the cytotoxicity and antitumor properties were performed. In vitro cytotoxicity (L1210 and Calc 18) shows a relationship between the cytotoxicity of these compds. and their topoisomerase poisoning properties. However, all these compds. were devoid of significant antitumor effect on the P388 murine leukemia system.
 IT 154283-53-1
 RL: RCT (Reactant); RACT (Reactant or reagent) (cytotoxicity and topoisomerase-inhibiting activity of)
 RN 154283-53-1 CA
 CN 1,2-Ethanediamine,
 N'-(2,3-dimethoxy[1,3]benzodioxolo[5,6-c]phenanthridin-13-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



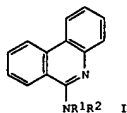
L8 ANSWER 12 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 119:117172 CA
 TITLE: Reaction of 2-acylcyclohexane-1,3-diones with 6-hydrazinophenanthridine
 AUTHOR(S): Rubinov, D. B.; Mikhailovsky, A. G.; Lahvich, F. A.
 CORPORATE SOURCE: Inst. Tekh. Khim., Perm, 614600, Russia
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (12), 1617-20
 CODEN: KGSSAQ; ISSN: 0132-6244
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

L8 ANSWER 12 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

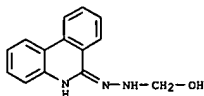


AB Condensation of cyclohexanediones I (R1 = Me, H, R2 = Me, Me(EtS)CHCH2, 1,3,5-Me3C6H2, R3 = H, CO2Me, R4 = Me, Pr, Cl1H23) with 6-hydrazinophenanthridine gave 79-91% enehydrazinoketones II; heating the reaction mixture caused cyclization to give 65-76% tetrahydroindazoles
 III [R1 = R2 = Me, R3 = H, R4 = Me, Pr; R1 = H, R2 = Me(EtS)CHCH2, R3 = H, R4 = Pr].
 IT 144402-92-6, 6-Hydrazinophenanthridine
 RL: RCT (Reactant); RACT (Reactant or reagent) (condensation of, with acylcyclohexanediones)
 RN 144402-92-6 CA
 CN 6(5H)-Phenanthridinone, hydrazone (9CI) (CA INDEX NAME)

L8 ANSWER 13 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 119:582 CA
 TITLE: Synthesis, antiaggregation, and antiarrhythmic activity of phenanthridine derivatives
 AUTHOR(S): Mikhailovsky, A. G.; Taranova, T. G.; Syropatov, B. Ya.; Vakhnin, M. I.
 CORPORATE SOURCE: Inst. Tekhn. Khim., Perm, Russia
 SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1992), 26(11-12), 53-5
 CODEN: KHFZAN; ISSN: 0023-1134
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

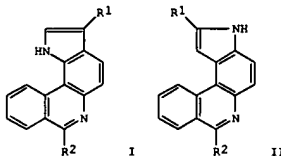


AB Phenanthridine derivs. (I, R1 = e.g., H, R2 = cyclohexyl, o-toluy, NR1R2 = morpholino) were prepared by the reaction of 6-chlorophenanthridine with the corresponding amines. I showed blood platelet aggregation inhibitory and antiarrhythmic activities in mice.
 IT 144402-93-7
 RL: BIOL (Biological study)
 (antiarrhythmic and blood platelet aggregation inhibitory activities of)
 RN 144402-93-7 CA
 CN 6(5H)-Phenanthridinone, (hydroxymethyl)hydrazone (9CI) (CA INDEX NAME)

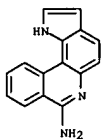


L8 ANSWER 14 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

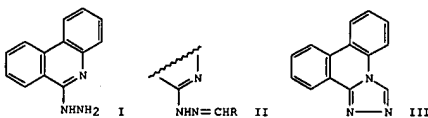
L8 ANSWER 14 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 118:38800 CA
 TITLE: Pyrrolophenanthridines. VI. Chemical properties of 1H-pyrrolo[2,3-a]phenanthridine and 3H-pyrrolo[3,2-a]phenanthridine
 AUTHOR(S): Samoilova, M. E.; Buyanov, V. N.; Baberkina, E. P.; Bezrukov, I. A.; Suvorov, N. N.
 CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, Russia
 SOURCE: Zhurnal Organicheskoi Khimii (1992), 28(4), 831-5
 CODEN: ZORKAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



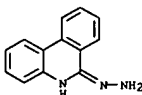
AB Pyrrolophenanthridines I and II (R1 = R2 = H) underwent electrophilic substitution (Vilsmeier, azo coupling, and Mannich reactions) and nucleophilic amination (Chichibabin reaction) to give the corresponding products I, II (R1 = CHO, p-O2NC6H4N; R2 = H; R1 = H, R2 = NH2) and I (R1 = Me2NCH2, R2 = NH2).
 IT 145163-19-5, 1H-Pyrrolo[2,3-a]phenanthridin-7-amine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reactions of)
 RN 145163-19-5 CA
 CN 1H-Pyrrolo[2,3-a]phenanthridin-7-amine (9CI) (CA INDEX NAME)



L8 ANSWER 15 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 117:233824 CA
 TITLE: Synthesis and properties of phenanthridine hydrazones
 AUTHOR(S): Mikhailovskii, A. G.; Shklyayev, V. S.
 CORPORATE SOURCE: Inst. Org. Khim., Perm, 614600, Russia
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (4), 531-4
 CODEN: KGSSAQ; ISSN: 0132-6244
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB 6-Hydrazinophenanthridine (I), prepared in 93% yield from the corresponding chloro derivative, condensed with RCHO (R = Cl3C, substituted Ph, 2-furyl) and CH2O to give hydrazone II, but condensation with HCO2H gave triazolophenanthridine III.
 IT 144402-92-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and condensation reactions with carbonyl compds.)
 RN 144402-92-6 CA
 CN 6(5H)-Phenanthridinone, hydrazone (9CI) (CA INDEX NAME)



L8 ANSWER 16 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 117:90108 CA

TITLE: Synthesis and alkylation of amidines of phenanthridine

AUTHOR(S): series

CORPORATE SOURCE: Mikhailovskii, A. G.; Vakhnin, M. I. Inst. Org. Khim., Perm, 614600, USSR

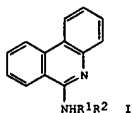
SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1991), (10), 1361-4

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



AB Amination of 6-chlorophenanthridine by $\text{R}_1\text{R}_2\text{NH}$ ($\text{R}_1 = \text{H}$, $\text{R}_2 = \text{PhCH}_2$; $\text{R}_1\text{R}_2 = (\text{CH}_2)_5$, $(\text{CH}_2)_{20}(\text{CH}_2)_2$) gave cyclic amidino derivs. I which were

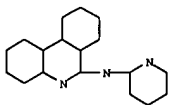
methylated by Me_2SO_4 to give the corresponding ammonium salts; similarly R_3NH_2 ($\text{R}_3 = \text{aryl}$) gave I ($\text{R}_1 = \text{H}$, $\text{R}_2 = \text{aryl}$). Depending on the structure of the starting amidine alkylation may proceed at the exocyclic (N-alkyl), phenanthridine (N-aryl), or pyridine (N-2-pyridyl) N atom; in the case of I ($\text{R}_1 = \text{H}$, $\text{R}_2 = 2\text{-pyridyl}$).

IT 88783-61-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and quaternization by Me iodide)

RN 88783-61-3 CA

CN 6-Phenanthridinamine, N-2-pyridinyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 17 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 116:173452 CA

TITLE: Resonance energies and tautomerism of substituted aromatic heterocycles and their benzo derivatives

AUTHOR(S): Yang, Pipeng; Duan, Wengui

CORPORATE SOURCE: Dep. Chem., Yunnan Univ., Kunming, 650091, Peop. Rep. China

SOURCE: Youji Huaxue (1991), 11(6), 620-3

CODEN: YCHHDX; ISSN: 0253-2786

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The recently developed quantified resonance theory (QRT) has been applied to substituted aromatic five- and six-membered heterocycles and their

benzo

derivs. The calculated resonance energy differences ARE between

tautomeric forms agree with those estimated from tautomeric equilibrium

data for

the 2- and 4-pyridone, 2-quinolone and 1-isoquinolone series. For

tautomerism of extensive heteroarom. compds. in solution, the ARE and

the differences in heats of atomization ΔH_A calculated by QRT can

be used to rationalize and predict the predominant tautomer and the

shifting trend in the equilibrium for a series of similar compds.

IT 832-68-8, 6-Phenanthridinamine

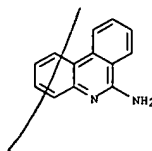
RL: PEP (Physical, engineering or chemical process); PRP (Properties);

PROC (Process)

(tautomerism of, resonance energy differences in)

RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 18 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 116:20919 CA

TITLE: Synthesis in the phenanthridine series. IV. Preparation of new radioprotectants with phenanthridine structure

AUTHOR(S): Lion, Claude; Boukou-Poba, Jean Paul; Charvy, Claude

CORPORATE SOURCE: Inst. Topol. Dyn. Syst., Univ. Paris 7, Paris, 75005, Fr.

SOURCE: Bulletin des Societes Chimiques Belges (1991), 100(2), 169-74

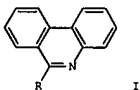
CODEN: BSCBAG; ISSN: 0037-9646

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 116:20919

GI



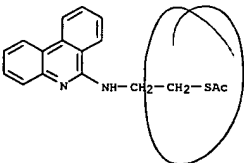
AB New phenanthridines I ($\text{R} = \text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_2\text{SAC}$, $\text{CH}_2\text{CH}_2\text{NMe}_2$, $\text{CH}_2\text{CH}_2\text{CH}_2\text{SAC}$, $\text{NHCH}_2\text{CH}_2\text{SAC}$ etc.) were easily obtained from I ($\text{R} = \text{Me}$) by a Mannich reaction, from I ($\text{R} = \text{Br}$) by substitution, or from I ($\text{R} = \text{CHO}$). These compds. are likely to be new radioprotectors.

IT 138118-78-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 138118-78-2 CA

CN Ethanethioic acid, S-[2-(6-phenanthridinylamino)ethyl] ester (9CI) (CA INDEX NAME)



L8 ANSWER 19 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 115:279858 CA

TITLE: Pyrrolophenanthridines. IV. Synthesis of 3H-pyrrolo[3,2-c]- and 3H-pyrrolo[3,2-a]phenanthridines. Reactivity of 3H-pyrrolo[3,2-c]phenanthridine

AUTHOR(S): Baberkina, E. P.; Samoilova, M. E.; Buyanov, V. N.;

CORPORATE SOURCE: Akhmediani, R. N.; Levina, I. I.; Bezzukov, I. A.;

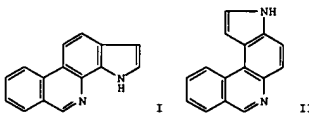
SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(5),

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



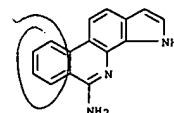
AB The nitration of mixture of 1- and 3-methylphenanthridines gave 1-methyl-2-nitro- and 3-methyl-4-nitrophenanthridines, which in turn afforded pyrrolophenanthridines I and II, resp., on treatment with $(\text{EtO})_2\text{CHNMe}_2$ in DMF in presence or absence of pyrrolidine, followed by cyclization with Zn/AcOH according to Lemgruber. II was also obtained in low yield in Fisher reaction from 2-aminophenanthridine. The aminomethylation, formylation and amination of I were studied.

IT 137531-26-1P, 3H-Pyrrolo[3,2-c]phenanthridin-5-amine

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 137531-26-1 CA

CN 3H-Pyrrolo[3,2-c]phenanthridin-5-amine (9CI) (CA INDEX NAME)



10/694,845

=> s l5 not l6

L7 78 L5 NOT L6

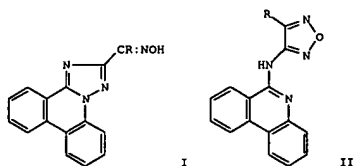
=> s l7 and py<1998

17927136 PY<1998

L8 77 L7 AND PY<1998

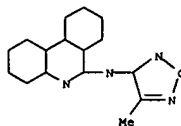
=> d ibib abs fhitstr 1-77

L8 ANSWER 20 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 113:191251 CA
 TITLE: A synthesis of 1,2,4-triazolo[1,5-f]phenanthridines
 by
 rearrangements of 1,2,5-oxadiazoles involving an NCN
 sequence with the imine nitrogen in an aromatic
 heterocyclic ring
 AUTHOR(S): Cusmano, Giuseppe; Macaluso, Gabriella; Gruttadauria,
 Michelangelo; Buscemi, Silvestre
 CORPORATE SOURCE: Dip. Chim. Org., Univ. Palermo, Palermo, 90123, Italy
 SOURCE: Heterocycles (1990), 31(5), 869-75
 CODEN: HETCYM; ISSN: 0385-5414
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 113:191251
 GI



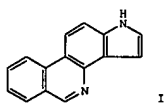
AB A synthetic pathway to the triazolophenanthridine system, e.g. (I; R =
 Me,
 Ph) by a base-catalyzed rearrangement of
 (phenanthridinylamino)oxadiazoles
 (II) has been investigated. This ring transformation is the first
 example
 of the applicability of the mononuclear heterocyclic rearrangement
 involving an NCN sequence to the synthesis of bridged nitrogen systems.
 IT 130137-89-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and base-catalyzed rearrangement of)
 RN 130137-89-2 CA
 CN 6-Phenanthridinamine, N-(4-methyl-1,2,5-oxadiazol-3-yl)- (9CI) (CA INDEX
 NAME)

L8 ANSWER 20 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

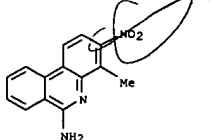


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

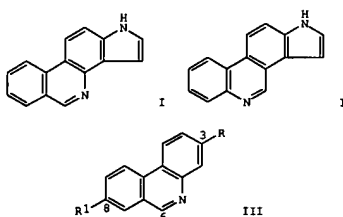
L8 ANSWER 21 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 113:78196 CA
 TITLE: Pyrrolophenanthridines. III. New method of
 1H-pyrrolo[2,3-c]phenanthridine synthesis
 AUTHOR(S): Baberkina, E. P.; Akhvlediani, R. N.; Buyanov, V. N.;
 Samoilova, M. E.; Levina, I. I.; Suvorov, N. N.
 CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
 SOURCE: Zhurnal Organicheskoi Khimii (1990), 26(2),
 445-50
 CODEN: ZORKAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 113:78196
 GI



AB 4-Methyl-3-nitro- (I), 2-methyl-1-nitro-, and 2-methyl-3-
 nitrophenanthridines were prepared by cyclization of 2-[(2-
 chlorobenzylidene)amino]-6- and 4-[(2-chlorobenzylidene)amino]-2-
 nitrotoluene on reaction with Na-NH3(1). Treating I with Me2NCH(OEt)2 in
 DMF-containing Et3N followed by reduction of the intermediate enamine by
 Zn-AcOH
 gave pyrrolophenanthridine II.
 IT 128422-33-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 128422-33-3 CA
 CN 6-Phenanthridinamine, 4-methyl-3-nitro- (9CI) (CA INDEX NAME)

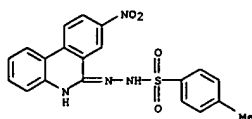


L8 ANSWER 22 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 107:236551 CA
 TITLE: Pyrrolophenanthridines. I. Synthesis and proton and
 carbon-13 NMR of 1H-pyrrolo[2,3-c]- and
 -[3,2-i]phenanthridines
 AUTHOR(S): Frolov, E. P.; Akhvlediani, R. N.; Krasnokutskii, S.
 N.; Kurkovskaya, L. N.; Suvorov, N. N.
 CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR
 SOURCE: Zhurnal Organicheskoi Khimii (1987), 23(1),
 189-95
 CODEN: ZORKAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 107:236551
 GI



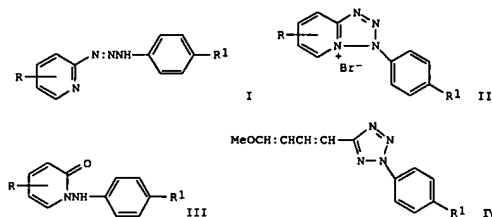
AB The novel heterocyclic comps. I and II were prepared from
 aminophenanthridines III (R = NH2, R1 = H; R = H, R1 = H2N) by successive
 diazotization-reduction with HONO-SnCl2 to give the corresponding
 hydrazine
 deriva., condensation with MeCOCO2H to give III (R, R1 = NHN:CMecO2H, H)
 and cyclization with ZnCl2. The starting III were prepared in 3 steps
 from
 the corresponding 3-nitro-6-chloro- and 8-nitro-6-chloro deriva.
 IT 111609-75-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and elimination reaction of)
 RN 111609-75-7 CA
 CN Benzenesulfonic acid, 4-methyl-, 2-(8-nitro-6-phenanthridinyl)hydrazide
 (9CI) (CA INDEX NAME)

L8 ANSWER 22 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



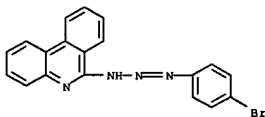
L8 ANSWER 23 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 107:39697 CA
 TITLE: Fused azolium salts. Part 8. Synthesis and nitrogen elimination of 3-aryltetrazolo(1,5-a)pyridinium salts and their angular benzenologs. Formation of N-arylamino- α -pyridones, -quinolones, -isoquinolones, and phenanthridones
 AUTHOR(S): Messmer, A.; Gelleri, A.; Hajos, Gy.
 CORPORATE SOURCE: Cent. Res. Inst. Chem., Hung. Acad. Sci., Budapest, H-1525, Hung.
 SOURCE: Tetrahedron (1986), 42(17), 4827-36
 DOCUMENT TYPE: CODEN: TETRA; ISSN: 0040-4020
 LANGUAGE: Journal
 OTHER SOURCE(S): English
 GI: CASREACT 107:39697



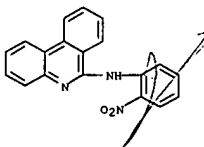
AB 2-Pyridylaryl triazenes I (R = H, 3-Me, 4-Me, 5-Me, 6-Me; R1 = H, OMe, Br, Cl) as well as 1-isoquinolyl-, 2-quinolyl and 6-phenanthridyl triazenes undergo cyclization in the presence of 2,4,6-tribromocyclohexa-2,5-dien-1-one to give 46-87% 3-aryltetrazolo(1,5-a)pyridinium salts II and their benzo analogs. These underwent N elimination with Et4N+OH- to give arylaminopyridinones III. Treatment of II with MeONa gave III together with the tetrazolylbutadiene esters IV.
 IT 108999-40-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and ring closure of)
 RN 108999-40-2 CA
 CN Phenanthridine, 6-[3-(4-bromophenyl)-1-triazenyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 23 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

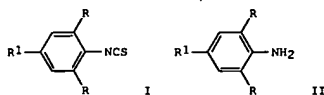


L8 ANSWER 24 OF 77 CA COPYRIGHT 2005 ACS on STN

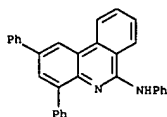
ACCESSION NUMBER: 104:19543 CA
 TITLE: Intramolecular reaction between nitro and carbodiimide
 groups: a new synthesis of 2-arylbenzotriazoles
 AUTHOR(S): Houghton, Peter G.; Pipe, David F.; Rees, Charles W.
 CORPORATE SOURCE: Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (7), 1471-9
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 104:19543
 AB On heating in a number of solvents, tetrazole I decomposed to give N, CO2, and 80-90% 2-phenylbenzotriazole (II). This rearrangement proceeds via (2-nitrophenyl)phenylcarbodiimide (III). A number of other precursors of III, and III itself, all gave II on heating. This reaction is general for all o-NO2-substituted diarylcarbodiimides and their precursors. The reaction mechanism involves a sequence of electrocyclic ring closing and opening reactions.
 IT 82937-37-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, reduction, and diazotization of)
 RN 82937-37-9 CA
 CN 6-Phenanthridinamine, N-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 25 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 102:112954 CA
 TITLE: Metathesis of aryl isothiocyanates: a novel method for the synthesis of sterically hindered aryl isothiocyanates
 AUTHOR(S): Habib, Nargues S.; Rieker, Anton
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.
 SOURCE: Synthesis (1984), (10), 825-7
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 102:112954
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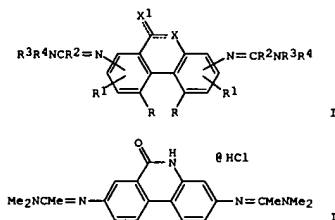


AB Isothiocyanates I (R = alkyl, Ph, iodo; R1 = alkyl, H, OMe, Ph, iodo) were prepared from anilines II and PhNCS. A mixture of II (R = R1 = Me) and PhNCS was refluxed to give I (R = R1 = Me) and some PhNHCSNHPh.
 IT 95096-34-79
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 95096-34-7 CA
 CN 6-Phenanthridinamine, N,2,4-triphenyl- (9CI) (CA INDEX NAME)



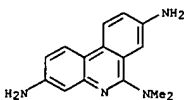
L8 ANSWER 26 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 102:6224 CA
 TITLE: Polycyclic bisamidines and their use as chemotherapeutic agents
 INVENTOR(S): Bajwa, Balbir Singh; Chatterjee, Dipak Kumar; Ganguli,
 PATENT ASSIGNEE(S): Bimal Naresh; Reden, Juergen; DeSouza, Noel John
 SOURCE: Hoechst A.-G., Fed. Rep. Ger.
 Ger. Offen., 31 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3305329	A1	19840823	DE 1983-3305329	19830217
EP 117467	A1	19840905	EP 1984-101373	19840210
EP 117467	B1	19870506		
R: CH, DE, FR, GB, IT, LI				
US 4599409	A	19860708	US 1984-580181	19840215
AU 8424660	A1	19840823	AU 1984-24660	19840216
JP 59163371	A2	19840914	JP 1984-26195	19840216
ZA 8401138	A	19840926	ZA 1984-1138	19840216
PRIORITY APPLN. INFO.:			DE 1983-3305329	A 19830217
OTHER SOURCE(S):			CASREACT 102:6224	
GI				

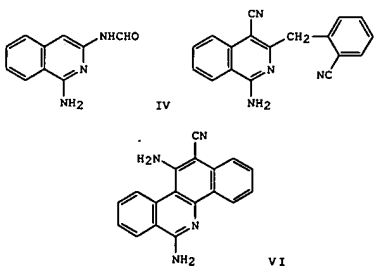


AB The title compds. (I: R = H, R2 = OC(O); R1 = H, alkyl, alkoxy, halo, NO2,

L8 ANSWER 26 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 amino; R2 = H, (un)substituted alkyl; R3, R4 = alkyl, R3R4N = heterocyclyl; X = O, N, NH; X1 = O, H, halo, alkoxy, amino, heterocyclyl; dotted lines represent optional double bonds] were prepd. Thus, 3,8 diamino-5(6H)-phenanthridinone was stirred 30 min at room temp. with POCl3/AcNMe2 to give 85% phenanthridinediylbis[acetamidine] II. I are effective in vitro protozoacides against Entamoeba histolytica at 50-200 mcg/L.
 IT 93494-47-4
 RL: RCT (Reactant); RACT (Reactant or reagent) (condensation of, with amides)
 RN 93494-47-4 CA
 CN 3,6,8-Phenanthridinetriamine, N6,N6-dimethyl- (9CI) (CA INDEX NAME)

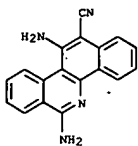


L8 ANSWER 27 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 99:175557 CA
 TITLE: Heterocyclic imines and amines. Part 18. Conversion of o-cyanobenzyl cyanide into isoquinoline, benzylisoquinoline, and azachrysene products
 AUTHOR(S): Bardard, Ian F.; Elvidge, John A.
 CORPORATE SOURCE: Chem. Dep., Univ. Surrey, Guildford, GU2 5XH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (6), 1137-40
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 99:175557
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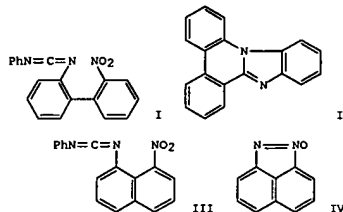


AB Treatment of 2-NCC6H4CH2CN (I) with NaNH2 in ice-cold HCONH2 under N2 for 2 h gave the dimers 2-NCC6H4CH(CN)C(NH)CH2C6H4CN-2 (II) and 2-NCC6H4CH(CN)C(NH)C6H4CH2CN-2 (III), and the HCONH2 adduct IV. II underwent cycloisomerization to give the isoquinoline V whereas III gave the benzo[c]phenanthridine VI. Treatment of I with NaOMe in refluxing MeOH for 8 h gave 9% V; a similar reaction in refluxing DMSO/MeOH for 2 h under N2 gave 44% V.
 IT 87606-65-39
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 87606-65-3 CA
 CN Benzo[c]phenanthridine-12-carbonitrile, 6,11-diamino- (9CI) (CA INDEX NAME)

L8 ANSWER 27 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

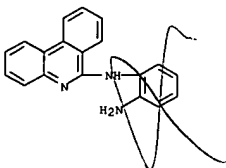


L8 ANSWER 28 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 97:127560 CA
 TITLE: New rearrangements in the pyrolysis of nitrocarbodiimides
 AUTHOR(S): Pipe, David F.; Rees, Charles W.
 CORPORATE SOURCE: Dep. Chem., Imp. Coll. Sci. Technol., London, SW7 2AY, UK
 SOURCE: Journal of the Chemical Society, Chemical Communications (1982), (9), 520-1
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 97:127560
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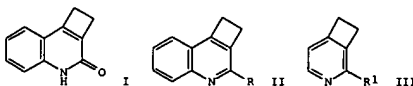


AB Flash vacuum pyrolysis of the nitrophenylcarbodiimide I gave 45% phenanthridine II, whereas similar treatment of the nitronaphthylcarbodiimide III gave 70% benzindazole N-oxide IV. Initially, intramol. nucleophilic attack by the O of the nitro group on the carbodiimide C occurs but the paths subsequently diverge to form 5-membered heterocyclic rings by different routes.
 IT 82937-38-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and diazotization of)
 RN 82937-38-0 CA
 CN 1,2-Benzenediamine, N-6-phenanthridinyl- (9CI) (CA INDEX NAME)

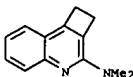
L8 ANSWER 28 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 29 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 97:55658 CA
 TITLE: Cycloadditions in syntheses. VIII. Synthesis of 1,2-dihydrocyclobuta[c]pyridine and -quinoline and their 3-substituted derivatives
 AUTHOR(S): Kaneko, Chikara; Naito, Toshihiko; Momose, Yu; Fujii, Harue; Nakayama, Nayomi; Koizumi, Ikue
 CORPORATE SOURCE: Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1982), 30(2), 519-25
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 97:55658
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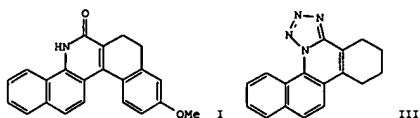
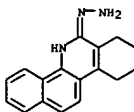


AB 1,2-Dihydrocyclobuta[c]quinolin-3(4H)-one (I) was prepared from 4-methoxyquinolin-2(1H)-one by photoaddn. of the latter to C2H4 and subsequent elimination of MeOH from the adduct. Chlorination of I with POCl3 gave 3-chloro derivative II (R = Cl), which then afforded either the parent base II (R = H) by reductive dechlorination, or 3-substituted derivs. II (R = MeO, MeS, Me2N, morpholino) by reaction with nucleophiles.
 The corresponding 1,2-dihydrocyclobuta[c]pyridine derivs. III (R1 = H, Cl, PhCH2O, MeO, EtS) were synthesized analogously.
 IT 82450-10-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 82450-10-0 CA
 CN Cyclobuta[c]quinolin-3-amine, 1,2-dihydro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 30 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 94:121256 CA
 TITLE: Synthesis of some heterocycles via enamines from 6-methoxy-1-tetralone and benzo[f]chroman-4-one
 AUTHOR(S): Sharma, S. D.; Manuja, Sushma; Gauba, A. L.
 CORPORATE SOURCE: Dep. Chem., Panjab Univ., Chandigarh, 160 014, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 19B(4), 246-9
 CODEN: IJSCDD; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 94:121256
 GI

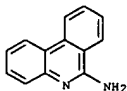
L8 ANSWER 30 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



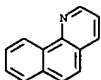
AB Reaction of 6-methoxy-1-tetralone and benzo[f]chroman-4-one with morpholine in the presence of $TiCl_4$ gives the resp. enamines in high yields. Treatment of these enamines with aryl isocyanates/isothiocyanates affords the corresponding lactams, e.g. I. I on refluxing with $POCl_3$ for 30 min gives fully aromatised 6-chloro-10-methoxydibenzo[c,k]phenanthridin e. Nucleophilic substitution of the halogen atom of 6-chloro-7,8,9,10-tetrahydrobenzo[c]phenanthridine with H_2NNH_2 yields the corresponding 6-hydrazino derivative, which on treatment with HNO_2 undergoes cyclization to give the benzotetrazolophenanthridine III.
 IT 76489-29-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of)
 RN 76489-29-7 CA
 CN Benzo[c]phenanthridin-6(5H)-one, 7,8,9,10-tetrahydro-, hydrazone (9CI) (CA INDEX NAME)

L8 ANSWER 31 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 89:191671 CA
 TITLE: Structural requirements for mutagenic activities of N-heterocyclic bases in the Salmonella test system
 AUTHOR(S): Matsumoto, Takashi; Yoshida, Daisuke; Mizusaki, Shigenobu; Tomita, Hideo; Koshimizu, Koichi
 CORPORATE SOURCE: Cent. Res. Inst., Japan Tob. and Salt Public Corp., Yokohama, Japan
 SOURCE: Agricultural and Biological Chemistry (1978), 42(4), 861-4
 CODEN: ABCHA6; ISSN: 0002-1369
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The mutagenic activities of quinoline [91-22-5], isoquinoline [119-65-3], phenanthridine [229-87-8], benzo[f]quinoline [85-02-9], benzo[h]quinoline [230-27-3], and their α -amino derivs. were compared in relation to the effects of structural changes using the S. typhimurium test system. All mutagenic compds. tested required the liver microsomal fraction for their mutagenic activity. Phenanthridine, two benzoquinolines, and quinoline were mutagenic. α -Amination of two benzoquinolines and quinoline increased their mutagenic activity intensively. Addition of a benzene ring to the benzene moiety of 2-aminoquinoline, so that two carbon atoms were shared, affected the increase in the mutagenic activity. Norhaman [244-63-3] increased the mutagenicity of 2-aminobenzo[f]quinoline [36193-75-6].
 IT 67419-74-3
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (mutagenicity of)
 RN 67419-74-3 CA
 CN 6-Phenanthridinamine, mixt. with benzo[h]quinoline (9CI) (CA INDEX NAME)
 CH 1
 CRN 832-68-8
 CMF C13 H10 N2

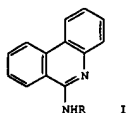
L8 ANSWER 31 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



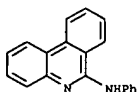
CH 2
 CRN 230-27-3
 CMF C13 H9 N



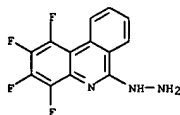
L8 ANSWER 32 OF 77 CA COPYRIGHT 2005 ACS on STN
 88:169929 CA
 TITLE: The cyclodeulfurization of thio-compounds. Part 15. Synthesis of 6-substituted aminophenanthridines from some thiourea derivatives
 AUTHOR(S): Omar, A. Mohsen M. E.; Habib, N. S.; Aboulwafa, M.
 CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt
 SOURCE: Pharmazie (1977), 32(12), 758-61
 CODEN: PHARAT; ISSN: 0031-7144
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 88:169929
 GI



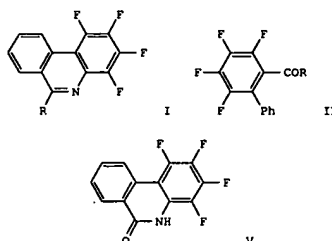
AB Phenanthridines I (R = 3-MeC₆H₄, 2-MeOC₆H₄, 4-ClC₆H₄, Ph, PhCH₂, Bu) were prepared by treating 2-PhC₆H₄NH₂ with RNCS and cyclizing 2-PhC₆H₄NHCSNHR with HgCl₂, POCl₃, or polyphosphoric acid. The best yields were obtained with POCl₃. The HgCl₂ complex of I-HCl (R = 3-MeC₆H₄) was also isolated.
 IT 846-62-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 846-62-8 CA
 CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)



L8 ANSWER 33 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

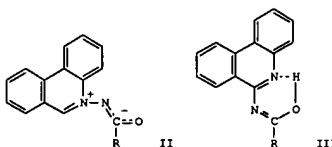


L8 ANSWER 33 OF 77 CA COPYRIGHT 2005 ACS on STN
 87:5778 CA
 TITLE: Synthesis of derivatives of 1,2,3,4-tetrafluorophenanthridine
 AUTHOR(S): Fomenko, T. V.; Gerasimova, T. N.; Fokin, E. P.
 CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR
 SOURCE: Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh Nauk (1977), (1), 99-102
 CODEN: IZSKAB; ISSN: 0002-3426
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI

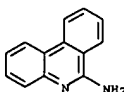


AB The phenanthridines I (R = Cl, piperidino, MNH₂, etc.) were prepared from II (R = OH), which was treated with SOCl₂, then with NaN₃ to give II (R = N₃) (III). Reaction of III with boiling EtOH, boiling C₆H₆/HCl, and CCl₄ (20°) gave 2-PhC₆F₄NHCO₂Et, (2-PhC₆F₄NH)2CO, and 2-PhC₆F₄NCO (IV), resp. Cyclization of IV with AlCl₃/PhCl gave V, which reacted with POCl₃ to give I (R = Cl) (VI). Treatment of VI with piperidine and hydrazine gave I (R = piperidino) and I (R = MNH₂), resp.
 IT 62799-19-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 62799-19-3 CA
 CN 6(5H)-Phenanthridinone, 1,2,3,4-tetrafluoro-, hydrazone (9CI) (CA INDEX NAME)

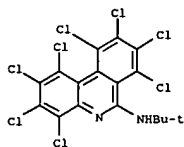
L8 ANSWER 34 OF 77 CA COPYRIGHT 2005 ACS on STN
 86:188776 CA
 TITLE: Electron deficient heteroaromatic ammonioamides. XII. The synthesis and photoisomerization of N-(5-phenanthridinyl)benzamides
 AUTHOR(S): Agai, B.; Lempert, K.; Hegedus-Vajda, J.
 CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Budapest, Budapest, Hung.
 SOURCE: Acta Chimica Academiae Scientiarum Hungaricae (1976), 91(1), 91-5
 CODEN: ACASA2; ISSN: 0001-5407
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 86:188776
 GI



AB Amination of phenanthridine with 2,4,6-Me₃C₆H₂SO₃NH₂ gave 5-aminophenanthridinium mesitylenesulfonate, acylation of which gave the 5-(diarylamino) analog (I). Partial dearylation of I gave II (R = Ph, 4-ClC₆H₄, 4-MeOC₆H₄, or 4-O₂NC₆H₄), which isomerized under UV irradiation to give the N-6-phenanthridinylbenzimidic acids III. The stability of III was due to N...HO H-bonding.
 IT 832-68-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



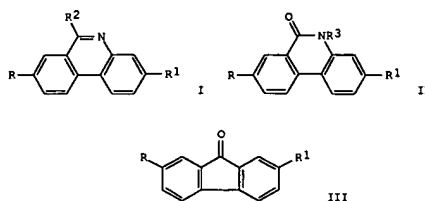
L8 ANSWER 35 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 85:94204 CA
 TITLE: Polyhaloheterocyclic compounds. Part XXIX.
 Perchloro-acridine, -phenanthridine, and
 -benzo[h]quinoline
 AUTHOR(S): Chambers, Richard D.; Daniels, Richard; Musgrave, W.
 Kenneth R.; Russell, Peter L.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (10), 1069-73
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 85:94204
 AB Perchloroacridine (I), -phenanthridine (II), and -benzo[h]quinoline were
 prepared by direct chlorination of the corresponding heterocycle or its
 monochloro derivative. Attempts to replace Cl by F were unsuccessful.
 Hydrolysis of I and II gave the 9-acridone and phenanthridin-6-one, resp.
 Nucleophilic substitution of I and II occurred at C-9 and C-6, resp.
 IT 60159-57-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrolysis of)
 RN 60159-57-1 CA
 CN 6-Phenanthridinamine, 1,2,3,4,7,8,9,10-octachloro-N-(1,1-dimethylethyl)-
 (9CI) (CA INDEX NAME)



L8 ANSWER 36 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 84:135502 CA
 TITLE: Phenanthridines and phenanthridinones as antiviral
 agents
 INVENTOR(S): Gauthier, George J.
 PATENT ASSIGNEE(S): Pfizer Inc., USA
 SOURCE: U.S., 13 pp. Division of U.S. 3,838,134.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

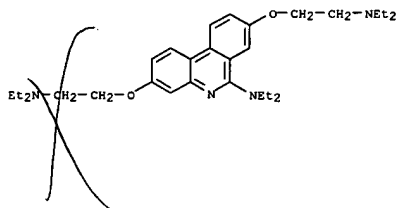
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3932643	A	19760113	US 1974-477529	19740607
US 3838131	A	19740924	US 1972-240830	19720403
US 3838134	A	19740924	US 1974-431255	19740107
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

GI

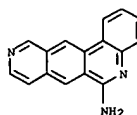


AB Phenanthridines I (R = R1 = Et2NCH2CH2O, (Me2CH)2NCH2CH2O; R2 = Cl, Et2N, PhCH2NH, MeO) and phenanthridinones II [R = H, R1 = Et2NCH2CH2O; R = Et2NCH2CH2O, R1 = H; R = R1 = Et2NCH2CH2O, Me2NCH2CH2CH2O, (Me2CH)2NCH2CH2O; R3 = H, Et2NCH2CH2O] were prepared. Ring expansion of fluorenone III by either a Schmidt reaction or a Beckmann rearrangement of its oxime gave II which was N-alkylated using R3X (X = halide) or was chlorinated using POCl3 and then condensed with R2H. Thus, III (R = R1 = Et2NCH2CH2O) was treated with HN3-H2SO4 to give II (R3 = H) (IV). IV when administered orally at 200 mg and 40 mg/kg to rats infected with

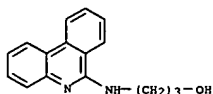
L8 ANSWER 36 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 encephalomyocarditis virus gave had 72% and 28% survival resp., whereas the known antiviral agent, III (R = R1 = Et2NCH2CH2O) gave survival rates of 93% and 49%, survival resp.
 IT 54153-44-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 54153-44-5 CA
 CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 37 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 84:121588 CA
 TITLE: Rearrangements in the photochemical synthesis of indolic compounds
 AUTHOR(S): Riche, Claude; Chiaroni, Angelo; Doucerain, Herve;
 Bessellievre, Richard; Thal, Claude
 CORPORATE SOURCE: Inst. Chim. Subst. Nat., Gif-sur-Yvette, Fr.
 SOURCE: Tetrahedron Letters (1975), (51), 4567-70
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB Irradiation of the indole I (R = CN, R1 = 1,2,5,6-N-methylpyridin-3-yl) in EtOH gave the spiroindole II and not a dihydroindole as previously stated (C. Deng, et al, 1975). The structure of II was determined by x-ray anal.
 The B and C rings in II formed an envelope conformation, with ring D in the semi-chair conformation of cyclohexene. II was a precursor of aspidospermane-type alkaloids. Irradiation of the indole I (R = CN, R1 = 4-pyridyl) in EtOH gave 7-(o-anilino)isoquinoline-6-carbonitrile (III) and the fused compds. IV and V. Irradiation of I (R = CN, CO2Me, R1 = 4-pyridyl) under oxidative conditions gave dehydro analogs of IV. The structure of III was determined by x-ray anal.
 IT 59171-78-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 59171-78-7 CA
 CN Pyrido[4,3-j]phenanthridin-6-amine (9CI) (CA INDEX NAME)



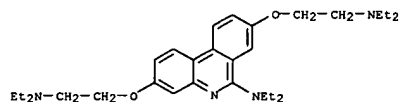
L8 ANSWER 38 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 84:4856 CA
 TITLE: Polycyclic fused amidines. I. Imidazo- and pyrimido[1,2-f]phenanthridines
 AUTHOR(S): Cookson, Ronald F.; Rodway, Ronald E.
 CORPORATE SOURCE: Nicholas Res. Lab., Slough, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1975), (19), 1850-4
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Phenanthridone (I; R = H) on heating with $\text{NH}_2(\text{CH}_2)_2\text{N}^+\text{H}_3$ p-MeC₆H₄SO₃- gave 2,3-dihydroimidazo[1,2-f]phenanthridine (III). The structure of II was confirmed by its synthesis from I (R = (CH₂)₂NH₂) by thermolysis. Imidazo[1,2-f]phenanthridine was prepared by dehydrogenation of II or by the
 the cycloaddn. of 6-chlorophenanthridine with $\text{NH}_2\text{CH}_2\text{CH}(\text{OMe})_2$.
 6-(3-Hydroxypropylamino)phenanthridine, on heating with POCl₃ gave 3,4-dihydro-2H-pyrimido[1,2-f]phenanthridine (III).
 IT 38052-91-4
 RL: RCT (Reactant); RACT (Reactant or reagent) (cyclization of)
 RN 38052-91-4 CA
 CN 1-Propanol, 3-(6-phenanthridinylamino)- (9CI) (CA INDEX NAME)



L8 ANSWER 39 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 81:169445 CA
 TITLE: Phenanthridinones as antiviral agents
 INVENTOR(S): Gauthier, George J.
 SOURCE: U.S., 11 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3838134	A	19740924	US 1974-431255	19740107
US 3838131	A	19740924	US 1972-240830	19720403
US 3932643	A	19760113	US 1974-477529	19740607
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

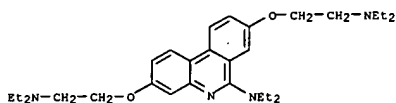
GI For diagram(s), see printed CA Issue.
 AB Phenanthridinones I [R = R₁ = OCH₂CH₂NET₂, O(CH₂)₃Me₂, OCH₂CH₂N (CHMe₂)₂; R = OCH₂CH₂NET₂, R₁ = H; R = H, R₁ = OCH₂CH₂NET₂; R₂ = H, Me, CH₂Ph, CH₂CH₂NET₂] were prepared by Schmidt reaction of the 9-fluorenones II with
 with NaN₃. Chlorination gave III (R₃ = Cl, R₄ = Et, CHMe₂), which were aminated or alkoxylated to III (R₃ = NET₂, NHCH₂Ph, OMe). Thus, Schmidt reaction of 5 g II (R = R₁ = CH₂CH₂NET₂) with 1.19 g NaN₃ gave 1.57 g I (R = R₁ = CH₂CH₂NET₂, R₂ = H), which at 40 mg/kg orally caused 28% survival in encephalomyocarditis virus-infected mice.
 IT 54153-44-5P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 54153-44-5 CA
 CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



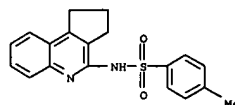
L8 ANSWER 40 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 81:152029 CA
 TITLE: Di(dialkylaminoalkoxy)phenanthridines as antiviral agents
 INVENTOR(S): Gauthier, George J.
 PATENT ASSIGNEE(S): Pfizer Inc.
 SOURCE: U.S., 11 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3838131	A	19740924	US 1972-240830	19720403
US 3838134	A	19740924	US 1974-431255	19740107
US 3932643	A	19760113	US 1974-477529	19740607
PRIORITY APPLN. INFO.:			US 1972-240830	A3 19720403
			US 1974-431255	A3 19740107

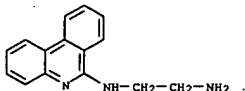
GI For diagram(s), see printed CA Issue.
 AB Phenanthridinones I [R = R₁ = OCH₂CH₂NET₂, O(CH₂)₃Me₂, OCH₂CH₂N (CHMe₂)₂; R = OCH₂CH₂NET₂, R₁ = H; R = H, R₁ = OCH₂CH₂NET₂; R₂ = H, Me, CH₂Ph, CH₂CH₂NET₂] were prepared by Schmidt reaction of the 9-fluorenones II with
 with NaN₃. Chlorination gave III (R₃ = Cl, R₄ = Et, CHMe₂) which were aminated or alkoxylated to give III (R₃ = NET₂, NHCH₂Ph, OMe). Thus, Schmidt reaction of 5 g II (R = R₁ = CH₂CH₂NET₂) with 1.19 g NaN₃ gave 1.57 g I (R = R₁ = CH₂CH₂NET₂, R₂ = H), which at 40 mg/kg orally caused 28% survival in encephalomyocarditis virus-infected mice.
 IT 54153-44-5P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 54153-44-5 CA
 CN 6-Phenanthridinamine, 3,8-bis[2-(diethylamino)ethoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



L8 ANSWER 41 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 79:146322 CA
 TITLE: Reactions between arenesulfonyl azides and tetrahydrocarbazoles
 AUTHOR(S): Bailey, A. Sydney; Buckley, Alan J.; Seager, John F.
 CORPORATE SOURCE: Dyson Perrins Lab., Univ. Oxford, Oxford, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (17), 1809-18
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The spiro compound (I) in F3CO₂H gave 1,2,3,4,4a,9a-hexahydro-9-methyl-4a-(p-tolylsulfonylamino)-9a-(trifluoroacetoxy)carbazolium trifluoroacetate which with Na₂CO₃ gave 2,3,4,4a-tetrahydro-9-methyl-4a-(p-tolylsulfonylamino)carbazole. The latter was an intermediate in the reaction of 4-MeC₆H₄SO₂N₃ and 9-methyltetrahydrocarbazole (II). Tetrahydrocarbazoles with arenesulfonyl azides in base gave cyclopentenoquinolines, e.g. II with 4-ClC₆H₄SO₂N₃ gave 80% imine (III). 1-Methyltetrahydrocarbazole with 4-Me- and 4-ClC₆H₄SO₂N₃ gave imine IV (R = Me and Cl, resp.). 1,9-Dimethyltetrahydrocarbazole with 4-MeC₆H₄SO₂N₃ gave sulfonamide V. The kinetics of the acid-catalyzed rearrangement of
 I were studied.
 IT 50527-99-6P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 50527-99-6 CA
 CN Benzenesulfonamide, N-(1,2,3,5-tetrahydro-4H-cyclopenta[c]quinolin-4-ylidene)-4-methyl- (9CI) (CA INDEX NAME)

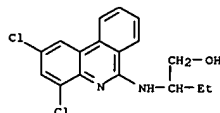


L8 ANSWER 42 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 78:124536 CA
 TITLE: Correction of: 77:88439
 AUTHOR(S): New synthesis of dihydroimidazo compounds
 CORPORATE SOURCE: Cookson, R. F.; Rodway, R. E.
 SOURCE: Nicholas Res. Inst., Slough/Bucks., UK
 Journal of the Chemical Society, Chemical
 Communications (1972), (9), 511-12
 CODEN: JOCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Phenanthridone or phthalazone was treated with H₂N(CH₂)₂NH₂.HS-
 O3CSH₄Me-p
 at 200-250° to give the dihydroimidazo-fused systems (I and II
 resp.).
 IT 40925-78-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 40925-78-8 CA
 CN 1,2-Ethanediamine, N-6-phenanthridinyl-, dihydrochloride (9CI) (CA INDEX
 NAME)



●2 HCl

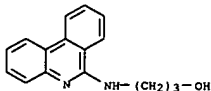
L8 ANSWER 43 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 77:139956 CA
 TITLE: Facile synthesis of 2,3-dihydroimidazo-and
 1,2,3,4-tetrahydropyrimido[1,2-f]phenanthridines
 AUTHOR(S): Pan, Hsi-Lung; Fletcher, T. Lloyd
 CORPORATE SOURCE: Sch. Med., Univ. Washington, Seattle, WA, USA
 SOURCE: Journal of Heterocyclic Chemistry (1972),
 9(4), 859-64
 CODEN: JHCTAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB When 6-(2-hydroxyethyl)amino-, 6-(3-hydroxypropyl)amino-, or
 6-[2-(1-hydroxybutyl)aminophenanthridines, dissolved in concentrated
 H₂SO₄,
 were treated with nitrosylsulfuric acid at 0-25°, then diluted with
 H₂O and basified with aqueous NaOH at 65-86°, 2,3-dihydroimidazo-,
 1,2,3,4-tetrahydropyrimido-, or 2,3-dehydro-2-ethylimidazo [1,2-f]
 phenanthridines (I, II, and III, R₁ = H, Cl, NO₂, R₂ = H, Cl, Br, R₃ = H,
 Cl, Br, NO₂, NH₂, R₄ = H, Cl, Br) were obtained resp. in good yields.
 Structures were substantiated by ir spectroscopy. The
 6-*m*-hydroxyalkylamino-phenanthridines were prepared from the
 6-chlorophenanthridines. A possible mechanism for the formation of these
 ring systems is postulated.
 IT 38040-74-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 38040-74-3 CA
 CN 1-Butanol, 2-[(2,4-dichloro-6-phenanthridinyl)amino]- (9CI) (CA INDEX
 NAME)



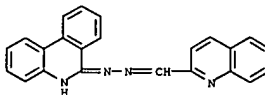
L8 ANSWER 44 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 77:126598 CA
 TITLE: Condensed nitrogen heterocycles
 INVENTOR(S): Rodway, Ronald Ernest; Cookson, Ronald Frederick
 PATENT ASSIGNEE(S): Aspro-Nicholas Ltd.
 SOURCE: Ger. Offen., 57 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2206012	A	19720824	DE 1972-2206012	19720209
GB 1347493	A	19740220	GB 1971-4457	19710211
CH 539643	A	19730914	CH 1972-1857	19720208
CH 539644	A	19730914	CH 1973-4310	19720208
BE 779128	A1	19720530	BE 1972-113762	19720209
FR 2125378	A5	19720929	FR 1972-4622	19720211
FR 2125378	B1	19750425		
US 3887566	A	19750603	US 1972-230464	19720229
SE 7413349	A	19741023	SE 1974-13349	19741023
PRIORITY APPLN. INFO.:			GB 1971-4457	A 19710211

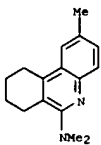
AB Comps. in the ring systems imidazo[1,2-a]quinoline, imidazo[2,1-a]phthalazine, imidazo[2,1-f]phenanthridine, imidazo[2,1-a]isoquinoline, imidazo[1,2-a]quinazoline, pyrimido[1,2-f]phenanthridine, indeno[1,2,3-de]pyrimido[2,1-a]phthalazine, imidazo[2,1-a]indeno[1,2,3-de]phthalazine, pyrimido[1,2-a]quinazoline, pyrimido[2,1-a]phthalazine, pyrimido[1,2-a]quinoline, pyrimido[1,2-a]quinoxaline, pyrimido[2,1-a]isoquinoline, imidazo[1,2-c]quinazoline (56) were prepared by
 ring-closure
 reaction of the *m*-chloroalkylheterocycles.
 IT 38052-91-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 38052-91-4 CA
 CN 1-Propanol, 3-(6-phenanthridinylamino)- (9CI) (CA INDEX NAME)



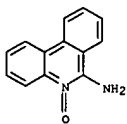
L8 ANSWER 45 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 76:135311 CA
 TITLE: Ligand structure and fluorescence of metal chelates.
 N-Heterocyclic hydrazones with zinc
 AUTHOR(S): Ryan, D. E.; Snape, F.; Winpe, M.
 CORPORATE SOURCE: Dep. Chem., Dalhousie Univ., Halifax, NS, Can.
 SOURCE: Analytica Chimica Acta (1972), 59(1), 101-6
 CODEN: ACACAM; ISSN: 0003-2670
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB -Benzimidazolecarboxaldehyde 2-quinolylhydrazone (I) is the most
 sensitive
 reagent of 15 N-containing heterocyclic hydrazones for the fluorimetric
 determination
 of Zn: <1 ppb Zn can be determined with excitation and emission
 wavelengths of
 470 and 520 nm, resp. Efficiency ratios (ER), which are a measure of the
 effect of nonradiative processes which compete with fluorescence from the
 excited state, are given: pyridine-2-aldehyde 2-pyridylhydrazone, which
 shows slight fluorescence with Zn, has an ER of 0.4 + 10-4 whereas
 I, which fluoresces strongly on reacting with Zn has an ER of 1.538
 + 10-7. Fluorescence intensity is greatest for those comps. which
 energetically prefer a -C=N- structural form.
 IT 35896-20-9D, 2-Quinolincarboxaldehyde, 6-
 phenanthridinylhydrazone, zinc complex
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (fluorescence spectrum of)
 RN 35896-20-9 CA
 CN 2-Quinolincarboxaldehyde, 6-phenanthridinylhydrazone (9CI) (CA INDEX
 NAME)



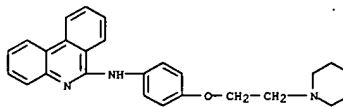
L8 ANSWER 46 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 76:85668 CA
 TITLE: Heterocyclic compounds. IV. Synthesis of some mono- and diazaphenanthrene derivatives
 AUTHOR(S): Bose, Ajay K.; Manhas, M. S.; Rao, V. V.; Chen, C. T.;
 CORPORATE SOURCE: Trehan, I. R.; Sharma, S. D.; Amin, S. G. Dep. Chem. Chem. Eng., Stevens Inst. Technol., Hoboken, NJ, USA
 SOURCE: Journal of Heterocyclic Chemistry (1971), 8(6), 1091-4
 CODEN: JHCTAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 76:85668
 GI For diagram(s), see printed CA Issue.
 AB 6-Chlorotetrahydrophenanthridines (I, R = H, 2-OMe, 2-Me, 2-Cl, 2-Br; R1 = Cl, NMe2, NHMe, NHet, H) were prepared as intermediates for the synthesis of antimalarials. A cyclohexanone enamine was treated with an aryl isocyanate to give quant. yields of enamides which gave ketoamides in acid. Cyclization yielded phenanthridones which reacted with POCl3 to give 6-substituted 7,8,9,10-tetrahydro-phenanthridines (I). Refluxing these products in an amide solution gave the N-substituted phenanthridines I (R = 4-Me, R1 = NHMe2, NHMe, NHet).
 IT 35417-80-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 35417-80-2 CA
 CN 6-Phenanthridinamine, 7,8,9,10-tetrahydro-N,N,2-trimethyl- (9CI) (CA INDEX NAME)



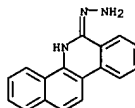
L8 ANSWER 48 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 66:104548 CA
 TITLE: Intramolecular trapping of hydroxylamines from the catalytic hydrogenation of 2-nitrobiphenyls
 AUTHOR(S): Muth, Chester W.; Elkins, J. R.; DeMatte, Michael L.; Chiang, S. T.
 CORPORATE SOURCE: West Virginia Univ., Morgantown, WV, USA
 SOURCE: Journal of Organic Chemistry (1967), 32(4), 1106-10
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 66:104548
 GI For diagram(s), see printed CA Issue.
 AB Catalytic hydrogenation of 2-nitro-2'-carboxybiphenyl (I) and its carboxy derivs. in ethanol in the presence of Pt has led to products resulting from the intramol. trapping of hydroxylamino and amino groups. In the presence of mineral acid the order of hydroxylamino trapping abilities is carbamoyl > carbomethoxy > carboxy. With no added mineral acid the order of trapping abilities is reversed. Compds. containing the cyano group were found to yield only hydroxylamino-trapped products.
 IT 7605-77-BDF, Phenanthridine, 6-amino-, 5-oxide, copper complex
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 7605-77-B CA
 CN Phenanthridine, 6-amino-, 5-oxide (6CI, 8CI) (CA INDEX NAME)



L8 ANSWER 47 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 75:108210 CA
 TITLE: Anticonvulsant activity of a series of phenanthridine basic ethers
 AUTHOR(S): Ashford, A.; Brown, G. R.; Palmer, P. J.; Ross, J. W.; Trigg, R. B.; Ward, R. J.
 CORPORATE SOURCE: Chem. Pharmacol. Sect., Twyford Lab. Ltd., London, UK
 SOURCE: Arzneimittel-Forschung (1971), 21(7), 937-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Twenty-two phenanthridine basic ethers (I), including 6-[m-(2-diethylaminoethoxy)phenyl]phenanthridine, 6-[p-(3-dimethylaminoethoxy)phenyl]phenanthridine, and 6-[p-(2-ethylaminoethoxy)phenyl]phenanthridine, showed potent anticonvulsant activity in mice against leptazol (II) and maximal electroshock convulsions, but neurotoxic activity was relatively high, precluding clin. use.
 IT 34244-46-7
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (antispasmodic activity of)
 RN 34244-46-7 CA
 CN Phenanthridine, 6-(β-piperidino-p-phenetidino)- (8CI) (CA INDEX NAME)



L8 ANSWER 49 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 64:104193 CA
 ORIGINAL REFERENCE NO.: 64:19603e-f
 TITLE: Dibenzo[c,h]cinnoline oxides
 AUTHOR(S): Poesche, W. H.
 CORPORATE SOURCE: Univ. Alberta, Edmonton, Can.
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (9), 890-3
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Dibenzo[c,h]cinnoline 5-oxide was synthesized. The compound is not identical with the H2O2 oxidation product of dibenzo[c,h]cinnoline and the Na2S reduction product of 1-nitro-2-o-nitrophenyl-naphthalene, which must therefore be dibenzo[c,h]cinnoline 6-oxide, as previously supposed.
 ASide from steric interactions, electronic effects are made responsible for the exclusive formation of the 6-oxide in the latter two cases.
 IT 6091-67-4, Benzo[c]phenanthridine, 6-hydrazino- (preparation of)
 RN 6091-67-4 CA
 CN Benzo[c]phenanthridine, 6-hydrazino- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 50 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 64:104192 CA

ORIGINAL REFERENCE NO.: 64:19603b-e

TITLE: Valence tautomerism of heterocycles. VII.

3,4-Diazabicyclo[4.2.0]octa-2,4-diene derivative

Maier, Guenther; Seidler, Friedrich

Tech. Hochsch., Karlsruhe, Germany

Chemische Berichte (1966), 99(4), 1236-40

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Cf. preceding abstrs. The preparation and properties of

1,6,7,8-tetramethyl-

2,5-diphenyl-3,4-diazabicyclo[4.2.0]octa-2,4-diene (I) are described.

1,2,3,4-Tetramethyl-3-cyclobutene-1,2-dicarboxylic anhydride (2.00 g.) in

AcOEt hydrogenated about 4 hrs. under ambient conditions over Pd-C

yielded

1.82 g. anhydride (III) of 1,2,3,4-tetramethyl-cyclobutane-cis-1,2-

dicarboxylic acid (III), m. 73-4° (petr. ether). II (2.00 g.)

dissolved at about 60° in a slight excess dilute aqueous NaOH, filtered,

and acidified with concentrated HCl precipitated 1.95 g. III, m. 150°

(Et2O-petroleum ether). III (2.00 g.) in 70 cc. dry Et2O stirred 16 hrs.

at room temperature with 5 mole equivs. PhLi-Et2O and poured into iced

H2O, and

the aqueous phase acidified with cold concentrated HCl gave 1.88 g. IV,

m.

140-1° (CHCl3-petroleum ether). IV (1.00 g.) in 20 cc. Et2O with

excess CH2N2-Et2O yielded 880 mg. Me 1,2,3,4-tetramethyl-cis-2-

benzoylcyclobutane-1-carboxylate (V), b.p. 140°. V (1.00 g.) and 3

cc. N2H4.H2O in 150 cc. EtOH refluxed 4 days while treated after 24 and

48

hrs. with addnl. 2-cc. portions N2H4.H2O gave 810 mg. VI, m. 207°

(EtOH). VI (1.00 g.) in 120 cc. dry tetrahydrofuran refluxed 3 hrs. with

3 mole equivs. PhLi-Et2O gave 760 mg. VII, m. 168° (AcOEt). VII

(750 mg.) in 50 cc. Ac2O kept 12 hrs. and poured with cooling into dilute

aqueous NaOH yielded 610 mg. yellow I, m. 174-5° (CH2Cl2-petroleum

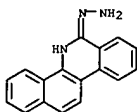
ether).

IT 6091-67-4, Benzo(c)phenanthridine, 6-hydrazino-

(preparation of)

RN 6091-67-4 CA

CN Benzo(c)phenanthridine, 6-hydrazino- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 52 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 63:24038 CA

ORIGINAL REFERENCE NO.: 63:4256e-f

TITLE: The phenanthridine series: preparation of some

methylphenanthridines and amino derivatives

Keene, B. R. T.; Tissington, P.

Medway Coll. Technol., Chatham, UK

Journal of the Chemical Society, Abstracts (

1965), (May), 3032-7

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1- and 10-Methyl and 1,10-dimethylphenanthridine have been synthesized.

Amination of these bases, and 1,2- and 9,10-benzophenanthridine, gave the

corresponding 6-amino derivatives. A partial resolution of

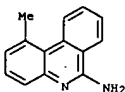
6-amino-1,10-dimethylphenanthridine has been achieved.

IT 1859-17-2, Phenanthridine, 6-amino-1-methyl-

(preparation of)

RN 1859-17-2 CA

CN Phenanthridine, 6-amino-1-methyl- (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 51 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 64:59793 CA

ORIGINAL REFERENCE NO.: 64:11173f-h, 11174a

TITLE: Heterocyclic derivatives of 2-chloroethyl sulfide

with

antitumor activity

Peck, Richard M.; O'Connell, Anna P.; Creech, Hugh J.

Inst. for Cancer Res., Philadelphia, PA

Journal of Medicinal Chemistry (1966), 9(2),

217-21

CODEN: JMCQAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Several monofunctional nitrogen and sulfur mustards (e.g. I-V) combined

with a variety of heterocyclic nuclei through aminoalkyl side chains were

synthesized for comparisons of their antitumor activities. The presence

of acridine, benzo(c)acridine, and phenanthridine nuclei increased the

antitumor effectiveness of both types of mustard moiety; the sulfur

mustard derivs. displayed higher, but much broader, dosage ranges of

activity. Since the sulfur mustards of 7-chloro- and 3,7-

dichloroquinoline were considerably more effective against Ehrlich

ascites

tumors in the mouse than the corresponding nitrogen half-mustards, it is

considered that studies utilizing sulfur mustard derivs. may be an

improved procedure for the detection of potential antitumor activity in

the carrier portion of the mol.

IT 4248-46-8, Phenanthridine, 6-[[3-[(2-chloroethyl)propylamino]propyl

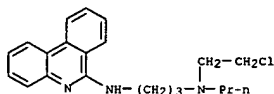
1]amino]-, dihydrochloride

(preparation of)

RN 4248-46-8 CA

CN 1,3-Propanediamine, N-(2-chloroethyl)-N'-6-phenanthridinyl-N-propyl-,

dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L8 ANSWER 53 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 62:10081 CA

ORIGINAL REFERENCE NO.: 62:1883g-h

TITLE: Symposium on molecular action of mutagenic and

carcinogenic agents. Acridine mutagens and DNA

structure

Lerman, L. S.

Med. Center, Univ. of Colorado, Denver

Journal of Cellular and Comparative Physiology (

1964), 64(2;Pt. II:Suppl. 1), 1-13, discussion

13-18

CODEN: JCCPAY; ISSN: 0095-9898

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Evidence for intercalation of acridine compds. between 2 otherwise

sequential base pairs was obtained by studies of sedimentation, low angle

x-ray scattering, flow dichroism, flowpolarized fluorescence, and

chemical

reactivity. Such binding requires a local untwisting and extension of

the

double helix. The intercalated mols. have a decreased chemical

reactivity.

They increase the stability of the double helix as shown by an increase

in

the thermal transition temperature Intercalation into complexes formed

between

polyadenylic and polyuridylic acids makes the double helix more stable

than the triple. Intercalation seems to be a prerequisite for

mutagenicity of the insertion-deletion type but the acridine structure is

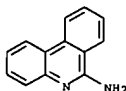
not essential and not all intercalating mols. are mutagenic.

IT 832-68-8, Phenanthridine, 6-amino-

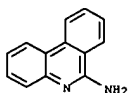
(deoxyribonucleic acid structure and)

RN 832-68-8 CA

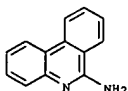
CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 54 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 62:3105 CA
 ORIGINAL REFERENCE NO.: 62:561d-e
 TITLE: Cyclic Amidines. XVII. 4-Imino-1,2,3-benzotriazines
 AUTHOR(S): Partridge, M. W.; Stevens, M. F. G.
 CORPORATE SOURCE: Univ. Nottingham, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1964), (Oct.), 3663-9
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 59, 5170e. 4-Imino-1,2,3-benzotriazines (I) afford, on reduction, 3-aminoindazoles (e.g. II) and on decomposition in acid, 6-aminophenanthridines. The reactions of o-cyanophenyltriazenes were studied.
 IT 832-68-8, Phenanthridine, 6-amino-
 (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

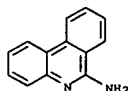


L8 ANSWER 55 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 (XI), m. 170°; the filtrate satd. with K2CO3 and extd. with Et2O, and the residue (1.7 g.) from the ext. triturated twice with 50-cc. portions hot 2N HCl left 70 mg. XI; the HCl ext. from the filter residue satd. with K2CO3 pptd. 3.5 g. V, m. 232-3°; the ext. from the 2nd fraction satd. with K2CO3, and extd. with Et2O yielded 0.6 g. III. I (0.03 mole) treated in the usual manner with 0.03 mole IV in 60 cc. dry C6H6, heated 2 hrs. at 60°, and hydrolyzed with cooling with 20 cc. H2O gave 2% VI and 95% unchanged IV.
 IT 832-68-8, Phenanthridine, 6-amino-
 (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

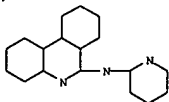


L8 ANSWER 55 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 58:33285 CA
 ORIGINAL REFERENCE NO.: 58:5635g-h, 5636a-d
 TITLE: Metal hydrazides. III. Amination of acridine and phenanthridine with sodium hydrazide and with sodium N,N-dimethylhydrazide
 AUTHOR(S): Kauffmann, Thomas; Hacker, Herbert; Mueller, Horst
 CORPORATE SOURCE: Tech. Hochschule, Darmstadt, Germany
 SOURCE: Ber. (1962), 95, 2485-92
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 58:33285
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 58, 2430f. The adducts from NaNHNH2 (I) or NaNHNMe2 (II) with acridine (III) or phenanthridine (IV) decomposed at 50-60° with elimination of NH3 or Me2NH, resp., and the formation of the Na salt of 9-aminoacridine (V) or 9-aminophenanthridine (VI), resp., in contrast to the corresponding adducts from C5H5N or isoquinoline (VII) which eliminate H under the same conditions. The adduct from III and II yields upon hydrolysis the surprisingly stable 9-(N,N-dimethylhydrazino)-9,10-dihydroacridine (VIII). All reactions with I and II were performed under pure N. Anhydrous Me2NNH2 (5.05 g.) treated with 3.65 g. NaNH2 in 70 cc. 90% C6H6 by the method previously described (CA 57, 7140h), the resulting suspension of 0.084 mole II treated dropwise with stirring at 0° with 5.0 g. III in 80 cc. C6H6, heated 4 hrs. at 60°, treated with 60 cc. H2O with cooling, and filtered yielded 5.4 g. (crude) V. III (5 g.) added with cooling to 0.084 mole II in the usual manner, stirred 2 hrs. with cooling, treated with cooling with 60 cc. H2O, and filtered, the filtrate extracted with Et2O, and the filter residue and Et2O extract worked up together gave 4.9 g. IX, m. 136-8° (Et2O at -60°), which kept 48 hrs. in a desiccator in vacuo decomposed to about 40% to III. II (0.084 mole) in 40 cc. C6H6-treated dropwise during a few min. with 5.0 g. IV in 100 cc. C6H6, heated 4 hrs. at 60°, hydrolyzed with 100 cc. H2O with cooling, and worked up yielded 4.6 g. VI, m. 195° (EtOH). II (0.03 mole) and 0.03 mole Me2NNH2 in 60 cc. C6H6 treated with 2.6 g. VII, heated 4 hrs. at 70°, hydrolyzed with cooling with 20 cc. H2O, and saturated with K2CO3, and the organic phase worked up yielded 2.5 g. 1-(N,N-dimethylhydrazino)isoquinoline, m. 86° (Et2O); monopicate m. 218-19° (EtOH). II (0.04 mole) in 80 cc. dry C6H6 treated at room temperature with a saturated solution of 2.0 g. 5,6-benzoquinoline in C6H6, heated 4 hrs. at 80°, and worked up gave 2.6 g. 2-(N,N-dimethylhydrazino)-5,6-benzoquinoline (X), m. 110° (petr. ether, b. 50-70°). 7,8-Benzoquinoline (3.6 g.) in C6H6 added at 5° to 0.06 mole II in 80 cc. dry C6H6, heated 3 hrs. at 80°, and worked up gave 3.6 g. yellow, viscous 7,8-isomer of X, b.p. 172-5°. III (5.0 g.) and 0.93 g. 99.2% N2H4 in 80 cc. C6H6 treated dropwise at 0° with 1.21 g. 90% NaNH2 in 70 cc. Et2O while being treated with a stream of N, heated 4 hrs. at 50°, treated with cooling with 50 cc. H2O, and filtered yielded 3.9 g. lemon-yellow crystals, m. 228-31°, which triturated 5 times with 50-cc. portions hot 2N HCl gave 89 mg. 9,10-dihydroacridine

L8 ANSWER 56 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 58:33284 CA
 ORIGINAL REFERENCE NO.: 58:5635e-g
 TITLE: Isothiocyanates. VIII. Study of the synthesis of diisothiocyanates and aminoisothiocyanates of acridine
 AUTHOR(S): Kristian, P.; Antos, K.; Hulka, A.; Nemecek, P.; Drobnica, L.
 CORPORATE SOURCE: Sloven. Vysoka Skola Tech., Bratislava, Czech.
 SOURCE: Chemické Zvesti (1961), 15, 730-6
 CODEN: CHZVAN; ISSN: 0366-6352
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. CA 56, 12854e. The problem of the synthesis of 1-isothiocyanato-5-aminoacridine, 2-isothiocyanato-5-aminoacridine, 3-isothiocyanato-5-aminoacridine and 2,8-diisothiocyanatoacridine from the corresponding diaminoacridines is described. Because of the unreactivity of the 5-NH2 group in 5-aminoacridine it was expected that the other NH2 group would be converted to isothiocyanate. For 1,5-(I), 2,5-(II) and 3,5-(III) diaminoacridine it was impossible to prepare the corresponding isothiocyanates. In I H bonds are formed between H on the hetero N with N of the 1-NH2 group. In II there is a possibility of the formation of a p-quinoid structure from 2-NH2 group with the ionized form of the acridonimine. In III there is a possibility of the formation of an amino-imine tautomeric structure of the 3-NH2 group. The synthesis of a new compound, 2,8-diisothiocyanatoacridine, m. 200°, by the thiophosgene method is described.
 IT 832-68-8, Phenanthridine, 6-amino-
 (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

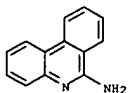


L8 ANSWER 57 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 58:3220 CA
 ORIGINAL REFERENCE NO.: 58:501h, 502a-b
 TITLE: The constitution of the red and colorless form of the quinolylmethanes. IV. Tautomerism and optical behavior
 of the quinolylamines
 AUTHOR(S): Credner, Hans H.; Friedrich, Hans J.; Scheibe, Guenter
 CORPORATE SOURCE: Tech. Hochschule, Munich, Germany
 SOURCE: Ber. (1962), 95, 1881-93
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. CA 57, 11162f. The quinolylamines, as did the corresponding methanes, existed in tautomeric forms and formed with suitable metal salts chelates which dissociated in basic solvents. The particular behavior of the proton was reflected in the absorption spectra. Di(2-pyridyl)amine (I) (4 g.) and excess MeI heated 2 hrs. at 90° in a sealed tube gave N,N'-dimethylpyridoazacyanine iodide (II), pale yellow needles, m. 290° (EtOH). I in absolute MeOH treated dropwise with stirring with 1 mole equivalent ZnCl₂ in MeOH gave I. ZnCl₂, m. above 360°. 9-Aminophenanthridine (III) (100 mg.) and 110 mg. 9-chlorophenanthridine (IV) fused together, boiled with alc. KOH, and filtered yielded 70% di(9-phenanthridyl)amine (V), yellow, m. 372° (HCONMe₂). IV (0.5 g.) and 0.34 g. 2-aminoquinoline (VI) heated together and worked up in the same manner gave 20% 2-quinolyl-9-phenanthridylamine (VII), yellow, m. 204° (EtOH). IV (0.5 g.) and 0.22 g. 2-aminopyridine (VIII) gave similarly yellow 2-pyridyl-9-phenanthridylamine (IX). The ultraviolet absorption spectra of VIII, I, I. ZnCl₂, VI, di(2-quinolyl)amine, N,N'-diethylquinoazacyanine iodide, III, IX, IX. ZnCl₂, VII, VII. ZnCl₂, V, V. ZnCl₂, and II were recorded and evaluated.
 IT 88783-61-3, Phenanthridine, 6-(2-pyridylamino)-(preparation of)
 RN 88783-61-3 CA
 CN 6-Phenanthridinamine, N-2-pyridinyl- (9CI) (CA INDEX NAME)



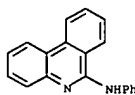
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 58 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



L8 ANSWER 58 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 55:144193 CA
 ORIGINAL REFERENCE NO.: 55:27316c-h
 TITLE: 6-Cyanophenanthridine and related compounds
 AUTHOR(S): Hayashi, Eisaku; Ohki, Hideya
 CORPORATE SOURCE: Shizuoka Coll. Pharm.
 SOURCE: Yakugaku Zasshi (1961), 81, 1033-6
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB 6-Cyanophenanthridine (I) (2 g.) in 30 ml. AcOH and 4 ml. 10.8% H₂O₂ heated 5 hrs. at 95-100°, cooled, and the product filtered off gave 2.1 g. I 5-oxide (II), needles, m. 216-17° (CHCl₃-MeOH). Catalytic reduction of 0.3 g. II in 10 ml. each of C₅H₅N and MeOH with Raney Ni gave 0.17 g. I, m. 136-7°. I (1 g.) in 20 ml. C₅H₅N and 15 ml. 10.8% H₂O₂ treated with 1 g. K₂CO₃ in 10 ml. H₂O and the product filtered off gave 0.9 g. 6-phenanthridinecarboxamide (III), needles, m. 190-2° (CHCl₃). II (1 g.) in 20 ml. C₅H₅N treated with 10 ml. 10.8% H₂O₂, 0.7 g. K₂CO₃, and 7 ml. H₂O, the mixture kept 1 hr. and the product filtered off gave 0.85 g. III 5-oxide (IV), needles, m. 283° (decomposition). III (0.5 g.) in 6 ml. AcOH and 1 ml. 10.8% H₂O₂ heated 5 hrs. at 95-100° and the product filtered off and washed with MeOH gave 0.25 g. IV, m. 283° (decomposition). I (0.4 g.) in 2.5 ml. concentrated H₂SO₄ and 0.2 ml. H₂O heated 1 hr. at 95-100°. H₂O added, and the mixture neutralized with NH₄OH gave 0.35 g. III, needles, m. 190-2°. Similarly, hydrolysis of 0.4 g. II yielded 0.4 g. IV, m. 283° (decomposition). I (1 g.) in 6 ml. concentrated H₂SO₄ and 0.5 ml. H₂O heated 1 hr. at 95-100°, the mixture cooled, treated dropwise with 0.5 g. NaNO₂ in 3 ml. H₂O, heated 30 min. at 95-100°, H₂O added, and the product filtered off gave 1.1 g. phenanthridine-6-carboxylic acid (V), needles, m. 158° (MeOH). II (0.6 g.) in 3.5 ml. concentrated H₂SO₄ and 0.3 ml. H₂O heated 1 hr. at 100° and the product filtered off gave 0.6 g. IV, m. 283° (decomposition). A solution of 0.4 g. KOH, 2 ml. H₂O, 0.3 g. Br, and 0.4 g. IV heated 20 min. at 80°, the precipitate taken up in 10% HCl, filtered with C, and neutralized with NH₄OH gave 0.25 g. 6-aminophenanthridine (VI), needles, m. 192-3°. Similarly, 0.6 g. IV yielded 0.15 g. VI 5-oxide, columns, m. 244-5°. V (0.4 g.) in 4 ml. AcOH and 0.8 ml. 10.8% H₂O₂ heated 5 hrs. at 100° gave 0.15 g. 6-hydroxyphenanthridine 5-oxide, m. 291-4° (C₅H₅N) and the mother liquor gave 0.1 g. phenanthridone, m. 288-90°. A mixture of 1.5 g. 6-phenoxyphenanthridine, 1.5 g. urea, and 5 g. PhOH heated 2 hrs. at 180°, cooled, 30 ml. 10% NaOH added, and the product filtered off gave 0.8 g. VI, m. 191-3°.
 IT 832-68-8, Phenanthridine, 6-amino-(preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 59 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 55:144186 CA
 ORIGINAL REFERENCE NO.: 55:27311i, 27312a-b
 TITLE: Reaction of phenanthridine 5-oxide with phenyl isocyanate
 AUTHOR(S): Hayashi, Eisaku
 CORPORATE SOURCE: Shizuoka Coll. Pharm.
 SOURCE: Yakugaku Zasshi (1961), 81, 1030-2
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Phenanthridine 5-oxide (I) (0.2 g.) in 10 ml. CHCl₃ heated with 0.12 g. PhNCO and the product extracted with (Me₂CH)₂O gave 0.15 g. 6-anilino-phenanthridine (II), plates, m. 152-4° (MeOH). 6(5H)-Phenanthridinone (5 g.) and 10 g. POCl₃ heated gradually up to 100°, the mixture kept 5 min. at 110-15°, cooled, the residue in 50 ml. CHCl₃ at 0° shaken with 40 ml. concentrated NH₄OH, the CHCl₃ layer passed through 16 ml. Al₂O₃, and the effluent concentrated gave 4.9 g. 6-chlorophenanthridine (III), needles, m. 116-17°; 3 g. I in 20 ml. CHCl₃ treated dropwise with 4 g. SO₂Cl₂, the mixture refluxed 5 min., and the product treated as above gave 2.8 g. III, m. 116-17°. III (6 g.) in 6 ml. C₆H₆, 6 g. PhOH, and 6 g. K₂CO₃ heated 2 hrs. at 100°, cooled, 15 ml. 10% NaOH added, the product extracted with 30 ml. CHCl₃, concentrated to 10 ml., and 10 ml. (Me₂CH)₂O added gave 7.1 g. 6-phenoxyphenanthridine (IV), columns, m. 116-17°. IV (1 g.) and 1.5 g. PhNH₂ heated 2 hrs. at 180°, cooled, and 1 ml. AcOH and 5 ml. H₂O added gave 0.7 g. II, m. 153-4° (MeOH).
 IT 846-62-8, Phenanthridine, 6-anilino-(preparation of)
 RN 846-62-8 CA
 CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)



LB ANSWER 60 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 54:62618 CA
 ORIGINAL REFERENCE NO.: 54:12077c-h
 TITLE: Some derivatives of 5,6,7,8-tetrahydrophenanthridine
 AUTHOR(S): Hollingsworth, B. L.; Petrow, V.
 CORPORATE SOURCE: Univ. London
 SOURCE: Journal of the Chemical Society, Abstracts (1960) 263-6
 CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE:

JOURNAL

LANGUAGE:

OTHER SOURCE(S):

AB cf. C.A. 43, 1778g. Cyclohexanone (100 g.), 18 g. H₂CO and 22 g. Et₂NH.HCl refluxed 6 min., then the crude product refluxed 16 hrs. with 16.5 g. p-H₂NC₆H₄CO₂Et, 20.2 g. p-H₂NC₆H₄CO₂Et.HCl and 40 g. SnCl₄.H₂O, the mixture cooled, basified, extracted with Et₂O and the extract in EtOH treated with picric acid gave Et 5,6,7,8-tetrahydrophenanthridine-3-carboxylate (I), m. 75°, as the picrate, m. 212-13°; saponification of I gave the acid, m. 312°, converted with POCl₃-PCl₅ to the acid chloride (II), and this to the amide (III), m. 250-2°. III (1 g.) added to an ice-cold solution of 1 g. Br in 12 ml. 10% KOH, the mixture kept 45 min. at 0°, 8 ml. 10% KOH added, the mixture heated 30 min. on a water bath, then chilled yielded 0.45 g. 3-amino-5,6,7,8-tetrahydrophenanthridine, m. 168-70° (benzamide m. 224-5°). II with NHEt₂ in C₆H₆ gave the 3-diethylamino analog, m. 100-1°, and the 3-dimethylamino analog (IV), m. 95-6° (picrate m. 250-1°), was similarly prepared from N,N-dimethyl-p-phenylenediamine. 3-Methoxy-5,6,7,8-phenanthridine (3 g.) refluxed 2 hrs. with 15 ml. constant boiling HBr

and worked up gave 2.5 g. 3-hydroxy analog of IV, m. 288-9° (picrate m. 221-3°; benzoate m. 138-9°). IV (4 g.), 15 ml. PhNEt₂ and 4 g. NaNH₂ heated 4 hrs. at 160°, the black precipitate taken up in 3% ACOH

and basified yielded 9-amino-3-dimethylamino-5,6,7,8-tetrahydrophenanthridine, m. 185-7° (acetate salt m. 222-3°). 2-Methyl-5,6,7,8-tetrahydrophenanthridine, m. 57° (picrate m. 231-2°), was prepared from m-H₂NC₆H₄Me and the 3-chloroanalog, m. 90° (10-oxide m. 169-70°; nitrate m. 152-3°), was prepared from p-ClC₆H₄NH₂. 5,6,7,8-Tetrahydrophenanthridine (V) nitrate, m. 156-7°, (3.3 g.) added to 6 ml. H₂SO₄ and 4 ml. 30% oleum at 0°, kept 30 min. at 0°, heated 1 hr. on a water bath, poured into H₂O and neutralized precipitated the

4-nitro derivative of V, m. 119-20°, and this reduced and benzooylated gave the 4-benzamido analog, m. 149-50°. 2-Phenyliminomethylcyclohexanone (50 g.) refluxed 20 hrs. with 400 ml. HCO₂H, the mixture concentrated, poured into aq NH₃ and the base purified through

the picrate gave 20% 2-anilinomethylcyclohexanone (VI), m. 88-9° (picrate m. 228-9°). VI (5 g.), 4 g. PhNH₂ and 5 g. SnCl₄ in 100 ml. alc. refluxed 8 hrs. gave 70% V, m. 63°. IT 100949-91-5, Phenanthridine, 6-amino-2-dimethylamino-7,8,9,10-tetrahydro- (preparation of)

LB ANSWER 61 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 54:14675 CA
 ORIGINAL REFERENCE NO.: 54:28931,2894a-c
 TITLE: Heats and entropies of ionization of some aromatic and N-heteroaromatic amines
 AUTHOR(S): Elliott, J. J.; Mason, S. F.
 CORPORATE SOURCE: Univ. Exeter, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1959) 2352-9
 CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE:

JOURNAL

LANGUAGE:

AB The ionization consts. of a series of unsubstituted polycyclic aromatic amines were measured at 0 and 20° in 50% EtOH-H₂O solution, and those of a series of N-heteroaromatic amines at 5 and 35° in H₂O. Entropies and enthalpies of ionization were calculated. The compds.

studied were PhNH₂; o-, m-, and p-NH₂C₆H₄Ph; 2-aminofluorene; 1- and 2-naphthylamine; 1-, 2-, 3-, and 9-phenanthrylamine; 1-, 2-, and 9-anthrylamine; 3-aminopyrene; 2-, 3-, and 4-aminopyridine; 2-, 3-, 4-, 5-, 6-, 7-, and 8-aminquinoline; 1-, 3-, 4-, 5-, 6-, 7-, and 8-aminoisoquinoline; 1-, 2-, 3-, 4-, and 5-aminoacridine; 6- and 9-aminophenanthridine; 2-amino-4-methyl-5,6-, 1'- and 4'-amino-5,6-, 3-amino-6,7-, and 2-amino-4-methyl-7,8-benzoquinoline; 8-amino-1,2-, and 8-amino-3,4-benzacridine. The variation in the ionization consts. of the aromatic amines is due equally to the entropy and the enthalpy factor, whereas the variation in the N-heteroaromatic series is due primarily to enthalpy changes. The dissociation entropies of the conjugate acids of the

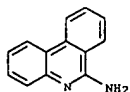
periaromatic amines are larger than those of the unhindered isomers, which in turn have larger values than those of the N-heteroaromatic amines.

These results are discussed in relation to the solvation of the amine cations and the π -electron energy changes accompanying their dissociation

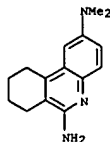
IT 832-68-8, Phenanthridine, 6-amino- (ionization of)

RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



LB ANSWER 60 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 RN 100949-91-5 CA
 CN Phenanthridine, 6-amino-2-dimethylamino-7,8,9,10-tetrahydro- (6CI) (CA INDEX NAME)



LB ANSWER 62 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 53:76177 CA
 ORIGINAL REFERENCE NO.: 53:13779i,13780a-b
 TITLE: The tautomerism of N-heteroaromatic amines
 AUTHOR(S): Mason, S. F.
 CORPORATE SOURCE: Univ. Exeter, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1959) 1281-9
 CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE:

JOURNAL

LANGUAGE:

OTHER SOURCE(S):

AB Infrared spectroscopy was used to study imine-amine tautomerism. The frequencies, extinction coeffs., and band half-widths of the absorption bands due to the N-H stretching vibrations of 23 primary and 7 secondary tri- and tetracyclic N-heteroaromatic amines and imines in dilute CCl₄ solution

were measured in the 3- μ region. The imines absorbed weakly near 3300 cm.⁻¹; the amines absorbed 5 to 10 times as intensely at slightly higher frequencies. These spectral differences were used to show that most of the tetracyclic and all of the tricyclic amines studied exist primarily

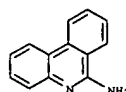
as the amino tautomer; an exception was 5-amino-2,3-benzacridine which exists mostly in the imino form. A review of ultraviolet data and an

examination of the ionization constant for 5-aminoacridine concurred with the infrared finding that this compound exists in the amino form.

IT 832-68-8, Phenanthridine, 6-amino- (spectra of, tautomerism and)

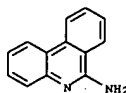
RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



L8 ANSWER 63 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 52:82602 CA
 ORIGINAL REFERENCE NO.: 52:14621f-1
 TITLE: Tautomerism and steric properties of 9-substituted phenanthridines
 AUTHOR(S): Reese, C. B.
 CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1958) 895-9
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB The amino form of 9-aminophenanthridine (I) (C.A.: 6-aminophenanthridine) was found to predominate in aqueous-alc. solution. The tautomeric equilibrium of the isomeric 5-aminoacridine is considered in comparison. The ultraviolet absorption spectra of the MeI salts of 1, 9-methylamino- (II), and 9-dimethylaminophenanthridine (III) were examined. Phenanthridone (IV) was shown to adopt the lactam form in alc. 9-Chlorophenanthridine (V) (3 g.) and MeOH saturated with 8 cc. NH₃ at 0°, heated 5 hrs. at 180°, the solvent removed, the residue extracted with H₂SO₄, and the extract neutralized gave 1.6 g. I, sublimed at 140°/0.5 mm., m. 193-5°. I (0.31 g.) and 1 cc. MeI heated 4 hrs. at 125° gave I.MeI (VI), m. 257° (MeOH), in quant. yield. VI (0.25 g.) suspended in 50 cc. CHCl₃, shaken with 10 cc. 3N aqueous NaOH until the turbidity in the aqueous layer disappeared, the CHCl₃ layer dried, the solvent removed, and the brown gum azeotropically distilled gave 0.065 g. crude 9,10-dihydro-9-imino-10-methylphenanthridine, which, purified by "cold finger" distillation at 110°/0.5 mm., m. 92°. II prepared by a known method m. 187-8°. V (1 g.) heated 2 hrs. at 100° with 2 g. pure anhydrous NHMe₂, the excess amine evaporated, the residue extracted with C₆H₆, and the solvent removed gave a gum in quant. yield; recrystn. yielded III which b.p. 119°, m. 60°. II (0.31 g.) quaternized with excess MeI as above gave the methiodide hemihydrate, m. 223-4° with darkening and effervescence. Similarly, III gave the methiodide, m. 222° (decomposition). V (0.21 g.) in 30 cc. anhydrous MeOH treated under reflux 0.5 hr. with NaOMe (from 0.1 g. Na) and 8 cc. MeOH, the solvents removed, the C₆H₆ extract evaporated, and the residue subjected to a "cold finger" distillation gave 9-methoxyphenanthridine (VII), b.p. 108°, m. 52°. The curve for IV was like that of 10-methylphenanthridone but quite unlike VII. The spectral curves for many of the above compds. are given.
 IT 832-68-8, Phenanthridine, 6-amino- (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 63 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)



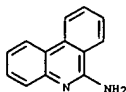
L8 ANSWER 64 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 52:55935 CA
 ORIGINAL REFERENCE NO.: 52:10095e-1, 10096a-i, 10097a-g
 TITLE: Aminoisoquinolines, -cinnolines, and -quinazolines. (A) The basic strengths and ultraviolet absorption spectra. (B) Infrared spectra
 AUTHOR(S): Osborn, A. R.; Schofield, K.; Short, L. N.
 CORPORATE SOURCE: Washington Singer Labs., Exeter, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1956) 4191-206
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. following abstract Potentiometric titrations in aqueous solution at 20° with HCl gave the following pKa values. Isoquinolines: unsubstituted (I), 5.40; 3-NH₂ (Ia), 5.05; 4-NH₂ (Ib), 6.28; 5-NH₂ (Ic), 5.59; 6-NH₂ (Id), 7.17; 7-NH₂ (Ie), 6.20; 8-NH₂ (If), 6.06. Cinnolines: unsubstituted (II), 2.29; 3-NH₂ (IIa), 3.70; 4-NH₂ (IIb), 6.85; 5-NH₂ (IIc), 2.70; 6-NH₂ (IId), 5.04; 7-NH₂ (IIe), 4.85; 8-NH₂ (IIIf), 3.68. Quinazolines: unsubstituted (III), 3.51; 2-NH₂ (IIIa), 4.82; 4-NH₂ (IIIf), 5.85; 5-NH₂ (IIIf), 3.57; 6-NH₂ (IIId), 3.29; 7-NH₂ (IIIe), 4.60; 8-NH₂ (IIIf), 2.81. In addition pKa values based on calcs. from ultraviolet extinction curves were determined for phenanthridine 4.52, its 6-NH₂ derivative 6.88, and 6,7-benzquinazoline (IV) approx. 5.2. Ultraviolet absorption data for the above bases and their cations in buffered aqueous solns. and of the methochlorides of I, II, and III in H₂O were given. I, II, and III showed the 3 main bands characteristic of electronic transitions parallel to the long, short, and long axes of bicyclic systems, and the effect of the position of the NH₂ substituent could be correlated fairly well with the shifts of the bands noted in the spectra of their NH₂ derivs. II in cyclohexane showed an addnl. low-intensity, longer wavelength (390 mμ) band of an n → π transition which disappeared in water or acid. The bathochromic shift shown in the spectra of the aminoisoquinolines on conversion to the cations indicated that, as with I, the monocations carry the proton on the ring N. Study of the ApKa values (relative to I) showed values below 1 for Ib, Ic, and Ie, in which there is no possibility of addnl. ionic resonance in the cations, and above 1 for the 1-NH₂ derivative of I and Id, for which addnl. forms are possible, and a neg. value for Ia, which is clearly not increased in stability by a possible o-quinonoid resonance form (see the following abstract for If). The bathochromic shifts in the spectra of the aminoisoquinolines on cation formation again indicated that proton attachment is to the ring N. By analogies to the quinoline and isoquinoline series, ApKa values indicated that N1 is the predominant basic center in IIb, IIe, and probably IIf, while N2 is the basic center for IId and IIf (the spectra of IIf and IIf are similar). From the values of ApKa for IIa, the basic center is considered to be N2, although it contrasts strongly with Ia. Cationization of III caused a marked hypsochromic shift in contrast to the more usual slight bathochromic shift for other heterocyclic bases, and

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 some modification of the aromatic system, possibly a 3,4-hydration, is assumed. Ultraviolet studies on cation formation of the aminoquinazolines indicated no hydration for IIIa and IIIb (similar to 2- and 4-aminoquinoline), IIIc, IIIf, and IIIf, while IIId is presumably hydrated. Considering the change on cationization of III and the increased base strength of 3,4-dihydroquinazolines relative to the quinazolines, choice of a basic center by correlation with ApKa values is difficult, although N1 seems to be favored for IIIb and definite for IIIf. Quinoxaline and its 6-NH₂ deriv. also showed the usual bathochromic shift on cation formation, while the 5-NH₂ deriv. seemed to take up the first proton on its NH₂ group. Infrared N-H bond stretching frequencies and force constants, indicative of the amt. of interaction of the NH₂ group with the ring and the electron density at the ring N, were given for Ia-f, IIa-f, IIIa-f, 2-, 4-, and 5-aminopyrimidines, and 5-aminoquinoline in CCl₄, CHCl₃, and pyridine (some compds.); the effects of electronic interaction where possible, the lack of interaction between N1 and a C-5 NH₂ group, the effect of 2 ring N atoms adjacent to the NH₂ group and of intramolecular H-bonding were noted. 1,3-Dichloroisoquinoline (0.5 g.), 25 cc. MeOH, 0.4 g. KOH, and 3 cc. Raney Ni shaken with H, the MeOH evapd., and the Et₂O ext. of the residue treated with picric acid in Et₂O gave I picrate, m. 225-6°; 1,3-dibromoisoquinoline (V) behaved similarly. Homophthalimide (5 g.) and 50 cc. PBr₃ refluxed 5 hrs., the PBr₃ evapd. in vacuo, and the residue treated with alkali gave 3.4 g. V, m. 147-7.5° (MeOH). V (3 g.) was converted to 1.75 g. 3-bromoisoquinoline (VI), m. 63-4° (aq. MeOH). 3-Chloroisoquinoline (8.8 g.), 100 cc. concd. NH₄OH, and 1 g. CuSO₄ heated 30 hrs. at 140° in an autoclave, made strongly basic, and extd. with CHCl₃ gave 5.3 g. Ia, m. 176-7° (C₆H₆), similarly prepd. from VI. Ib m. 108-9.5° (C₆H₆-cyclohexane). 5-Nitroisoquinoline (20 g.), 500 cc. MeOH, and 2 g. 5% Pd-C hydrogenated 2 hrs., evapd., and the residue crystd. from CHCl₃-petr. ether gave 931 Ic, m. 129.5-30.5° (C₆H₆-cyclohexane). m-MeOC₆H₄CHO (35.5 g.), 18 g. MeNO₂, 125 cc. HOAc, and 12.5 g. NH₄OAc refluxed 2 hrs. and poured into H₂O gave 27 g. m-MeOC₆H₄CH=CHNO₂, m. 91-2° (C₆H₆), which was not reduced satisfactorily. 1,2,3,4-Tetrahydro-6-methoxyisoquinoline (2.42 g.) and 0.8 g. 30% Pd-C heated 0.25 hr. at 180-90° in a stream of H, extd. with Et₂O, the 2.1 g. oily product treated with 3 g. picric acid in 10 cc. Me₂CO, the 2.9 g. picrate decompd. with aq. LiOH, extd. with Et₂O, the 1.03 g. product refluxed 2 hrs. with 25 cc. concd. HBr, evapd. in vacuo, dissolved in 10 cc. H₂O, and treated with aq. Na₂CO₃ gave 0.85 g. 6-hydroxyisoquinoline (VII), m. 220° (decomp.); dehydrogenation with Raney Ni in naphthalene was unsuccessful. Id, m. 211-12° (C₆H₆), was prepd. from VII. 1,3-Dihydroxy-7-nitroisoquinoline (VIII) (52 g.), m. 291° (decompn.), was prepd. from 56 g. 4-nitrohomophthalic acid in o-C₆H₄Cl₂. VIII (2 g.) and 20 cc. POCl₃ heated 4 hrs. on the steam bath, decompd. with ice, and brought to pH 10 gave 1.18 g. 1,3-dichloro-7-nitroisoquinoline, m. 185° (decompn.) (HOAc), but the reaction was not reproducible. 7-Hydroxyisoquinoline (1.25 g.), 4 cc. NH₄SO₃ (concd. NH₄OH satd. with SO₂), and 20 cc. concd. NH₄OH 16 hrs. at 140-50° gave 1.1 g. Ic, m. 203-5° (C₆H₆) after sublimation at 150°/0.3 mm. Ic (4.8 g.) in 12 cc. concd. HBr and 13 cc. H₂O diazotized at 0° with 2.3 g. NaN₂ in 15 cc. H₂O, added to 5.8 g. CuBr in 48 cc. HBr at 75°, and let stand 24 hrs. gave 5.1 g.

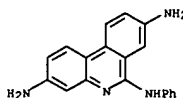
L8 ANSWER 64 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 5-bromoisoquinoline (IX), m. 82-4° (petr. ether). KNO₃ (2.4 g.) in 20 cc. concd. H₂SO₄ added during 5 min. to 4.15 g. IX in 24 cc. concd. H₂SO₄, the mixt. let stand 1 hr. at room temp., poured on ice, and made alk. with NH₄OH gave 5.05 g. 5-bromo-8-nitroisoquinoline (X), m. 139-41° (MeOH). 5-Chloro-8-nitroisoquinoline (2 g.) and 12 g. NH₄OH added to 2 g. 6% Pd-CaCO₃ in abs. MeOH (previously shaken with H₂), hydrogenated 1 hr., the filtered soln. acidified with concd. HCl, the MeOH evapd. in vacuo, the residue in H₂O made alk. with satd. Na₂CO₃, and extd. with CHCl₃ gave 1.02 g. If, m. 171-2° (EtOAc); use of NaOAc in the reduction gave lower yields of If while reduction with Pd-C in MeOH in the presence of NaOAc gave 8-amino-5-chloroisoquinoline, from which the Cl was not removed on Raney Ni hydrogenation in alk. soln.; hydrogenation of X in MeOH over Pd-CaCO₃ gave colored intermediate products, while reduction of X in the presence of KOH gave a small yield of If. 2-Chloroquinazoline (0.5 g.) added slowly to 0.4 g. KOH in 5 g. PhOH, the mixt. heated 3 hrs. at 70°, and made alk. gave 0.58 g. 2-phenoxyquinazoline (XI), m. 124-6° (petr. ether). XI (0.5 g.) and 5 g. NH₄OH heated 2 hrs. at 170-80° and treated with H₂O and 2N NaOH gave 0.35 g. IIIs, m. 200° (EtOH). IIIs m. 271-2° (EtOH). 6,2-DiN(H₂N)C₆H₃CO₂H (14.84 g.) and 29.4 cc. HCONH₂ 4.5 hrs. at 155-60° gave 12.2 g. 4-hydroxy-5-nitroquinazoline (XII), m. 252-6° (H₂O). XII (7 g.) and POCl₃ gave 5.17 g. 4-chloro-5-nitroquinazoline (XIII), m. 142° after sublimation at 140°/0.5 mm. Resublimed XIII (1 g.) in 150 cc. dry MeOH/2CH₂OH and 0.5 g. 6% Pd-CaCO₃ hydrogenated 0.5 hr., evapd., oxidized with K₃Fe(CN)₆, and the product chromatographed gave 0.265 g. IIIC, m. 195-6.5° (C₆H₆) after sublimation at 160°/1 mm. IIIC, m. 213-14° (C₆H₆), IIIC, m. 190-1° (C₆H₆) after sublimation at 160°/0.5 mm., and IIIC, m. 150-1° after sublimation at 120°/0.5 mm., were prep. similarly by reduction at atm. pressure with 6% Pd-C. 1-Chloro-7-methoxyphthalazine (XIV) (7.4 g.), m. 142° (decompn.), was obtained by refluxing 8.8 g. 1-OH compd. 0.5 hr. with 40 cc. POCl₃. XIV (0.5 g.), 0.2 g. red P, and 5 cc. HI refluxed 1 hr., dild. with 5 cc. H₂O, evapd. in vacuo, and the residue in 5 cc. H₂O adjusted to pH 7 with NH₄OH gave 0.3 g. 6-hydroxyphthalazine-0.5H₂O, m. 300° (decompn.) (H₂O), which was not converted successfully to the 6-NH₂ compd. XIV refluxed with H₂ gave 4,6-dihydroxyphthalazine, m. 310° (decompn.) (H₂O). 3,2-H₂NClO₆HO 2H (10 g.) was converted to 8.5 g. 4-hydroxy-6,7-benzoquinazoline (XV), m. 278° (H₂O). XV (1.3 g.) and 20 cc. POCl₃ refluxed 2 hrs. gave 0.98 g. 4-chloro-6,7-benzoquinazoline (XVI), m. 176-8° after sublimation at 160°/0.1 mm. XVI (0.4 g.) in 50 cc. MeOH/2CH₂OH hydrogenated 1.5 hrs. over 0.5 g. 8% Pd-CaCO₃ and the product in H₂O oxidized with 1.4 g. K₃Fe(CN)₆ gave 0.19 g. IV, m. 163-5° (cyclohexane) after sublimation. XVI (0.23 g.) and 25 cc. satd. NH₃-MeOH refluxed 2 hrs. gave 4-amino-6,7-benzoquinazoline, m. 365° (decompn.) (EtOH) after repeated sublimation. XVI (2.1 g.) in 100 cc. warm C₆H₆ added to 2 equivs. NaCH(CO₂Et)₂ in 100 cc. C₆H₆, refluxed 3 hrs., let stand

L8 ANSWER 65 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 ACCESSION NUMBER: 50:69424 CA
 ORIGINAL REFERENCE NO.: 50:13019c-1,13020a-e
 TITLE: New trypanocides. I. Quaternary salts derived from 2,7-diaminophenanthridine and the attempted preparation of quaternary salts from 2,7-diamino-9-anilino-phenanthridine
 AUTHOR(S): Davis, M.
 CORPORATE SOURCE: May & Baker Ltd., Dagenham, Essex, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1956) 337-43
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Salts of 2,7-diamino-(I) and 2,7-bis(ethoxycarbonylamino)-10-methylphenanthridine (II) were prepared by 2 routes.
 2,7-Diamino-9-anilino- (III) and 9-p-aminoanilino-phenanthridine (IV) were prepared from 9-chloro-2,7-dinitrophenanthridine (V). Attempts to convert III and IV into quaternary derivs. were unsuccessful. 2,7-Diaminofluorenone (31.3 g.) in concentrated H₂SO₄ cooled to -30° was treated during 1.25 h. below 0° with 21.8 g. NaN₃ in H₂O, 75 mL. H₂O added during the next 0.75 h., and the solution poured on ice and aqueous NH₃ to yield 26 g. 2,7-diaminophenanthridine (VI), m. 310-12° (decomposition) (from PhNO₂). Heating 1 g. VI with MeI in MeOH 24 h. at 115° gave 98% 2,7-bis(methylamino)phenanthridine-2-MeI.2H₂O (VII), m. 330-4° (decomposition), which on drying gave the monohydrate, and finally the anhydrous salt, λ_{0.1N} HCl 336, 325, and 260 mμ (ε 8200, 9700, and 23,300), λ_{inf} 1.269 mμ (ε 14,200). VI (24.3 g.), 25.8 mL. ClCO₂Et, 43 mL. PhNET₂, and 700 mL. EtOH refluxed 3 h. formed 33.6 g. 2,7-di(ethoxycarbonylamino)phenanthridine (VIII), prisms, m. above 360° (from dioxane). VIII (11.2 g.) refluxed 0.5 h. with 55 mL. POCl₃ gave 7.95 g. 9-chloro-2,7-bis(ethoxycarbonylamino)phenanthridine (IX), m. 252-4° (decomposition) (from EtOH). 2,7-Bis(ethoxycarbonylamino)-9-methylphenanthridine (10 g.) and 3.05 g. SeO₂ refluxed 7 h. in 400 mL. dioxane and 10 mL. H₂O yielded 7.45 g. 2,7-bis(ethoxycarbonylamino)-9-formylphenanthridine (X), m. 250-62° (decomposition). X (12 g.) heated at 50-5° in 157 mL. C₅H₅N, 3.7 g. KNO₃ in H₂O added during 1.5 h., after a further 1.5 h. at 50-5° the mixture was refluxed and filtered, and the residue extracted with hot C₅H₅N and K₂CO₃ solution. The C₅H₅N exts. were combined with the original filtrate, concentrated to 150 mL. and the carbonate extract added, the mixture refluxed, and filtered. The residue after further extraction with K₂CO₃ solution was 2.85 g. unchanged X. The combined exts. upon acidification gave 5.3 g. 2,7-bis(ethoxycarbonylamino)phenanthridine-9-carboxylic acid (XI) (5 g.) in 25 mL. PhNO₂ refluxed 2 h. gave 3.2 g. 2,7-bis(ethoxycarbonylamino)phenanthridine (XII), m. 250-3° (decomposition) (from alc.). IX (4 g.) suspended in 400 mL. hot alc. containing 1 g. KOH and Raney Ni was shaken with H₂, fresh catalyst added, and the suspension reheated gave 2.1 g. XII. On one occasion when 4 g. of IX was similarly reduced under pressure 2.85 g. of 2,7-bis(ethoxycarbonylamino)-9,10-dihydrophenanthridine was obtained, m. 192-4°; Ac derivative, m. 230-2°. XII (0.5 g.) heated 0.5 h. at 160° in concentrated H₂SO₄ and H₂O gave 2,7-diaminophenanthridine, m. 208-10° (decomposition). XII

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 overnight, poured into H₂O, the org. layer evapd., and the residue crystd. from EtOH gave 2.29 g. di-Et 6,7-benzoquinazolin-4-ylmalonate (XVII), m. 172-5°. XVII (1.5 g.), 0.6 g. KOH, and 60 cc. MeOH refluxed 3 hrs. gave 0.58 g. 6,7-benzoquinazolin-4-ylacetate, m. 207-9° (MeOH), hydrolyzed with boiling aq. NaOH to traces of 4-methyl-6,7-benzoquinazolin-1.5H₂O, m. 124-6° (petr. ether). I (5 g.), 10 cc. MeI, and MeOH refluxed 2 hrs. gave 1 methiodide, m. 160-1.5° (EtOH), which was shaken with 50 cc. H₂O and excess freshly pptd. AgCl for 12 hrs., filtered, the filtrate evapd., and 1 methochloride crystd. under anhyd. conditions from EtOH-Et₂O. Quinoline methochloride, the very deliquescent II methochloride-0.5H₂O, and 4-methylcinnoline methochloride-H₂O were prep. similarly.
 IT 832-68-8, Phenanthridine, 6-amino-
 (basicity and spectrum of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



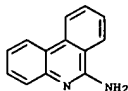
L8 ANSWER 65 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 (3.2 g.) in PhNO₂ treated 1 min. at 150° with 3.2 mL. Me₂SO₄ gave 4.15 g. of the Me methosulfate (XIII) of II as orange needles, decomp. above 280° from alc. (green fluorescence). XIII with KI in H₂O gave the methiodide (XIV) yellow needles, decomp. above 260° (from alc.). XIV was also obtained from the original base with MeI-MeOH. XIII (4.15 g.) heated 45 min. at 140° in H₂SO₄-H₂O yielded after treatment with KI 2.75 g. of the iodide (XV) of I. XV was similarly prep. from XIV as red needles, m. 288-90° (decompn.). Refluxing an aq. soln. of XV with freshly prep. AgCl gave the corresponding chloride, red prisms, m. 278-80° (decompn.). V (2 g.) and 9 mL. PhNH₂ refluxed 1 h. gave 2.2 g. 9-anilino-2,7-dinitrophenanthridine (XVI), orange prisms, m. 316-18°. V similarly afforded 93% 2,7-dinitro-9-p-nitroanilino-phenanthridine (XVII), decomp. 350-60° (from PhNO₂); Ac deriv., decomp. 300-4°. XVI (2.2 g.) refluxed 0.5 h. with 20 g. SnCl₂.2H₂O in 20 mL. concd. HCl gave 1.45 g. III as yellow plates, m. 225-6° (decompn.); hydriodide, orange needles, m. 224-6° (decompn.); tri-Ac deriv. (XVIII), m. 300-4° (from Et₂O-C₅H₅N). XVII similarly yielded 90% IV as yellow plates, m. 244-5° (decompn.); tri-Ac deriv. (XIX), m. 328-9° (decompn.); tetra-Ac deriv. (XX), decomp. 360°. IV (0.31 g.) in alc. refluxed 2 h. at 100° with 0.75 g. PhNET₂ and 0.55 g. ClCO₂Et gave 2,7-bis(ethoxycarbonylamino)-9-p-ethoxycarbonylaminoanilino-phenanthridine-HCl.2H₂O (XXI), m. 211-13° (decompn.); free base, m. 238-42° (from alc.). XVIII (0.6 g.), excess MeI, and MeOH refluxed 18 h. and left 3 days gave 0.63 g. of a salt, C₂₆H₂₅O₃N₄I (XXII), yellow plates, m. 330-40° (decompn.). XXII hydrolyzed with concd. HCl caused I to evolve and gave III, m. 224-6° (decompn.). XVIII (0.4 g.) similarly treated in a sealed tube 18 h. at 110° gave VII. IV (0.35 g.) with MeI-MeOH at 115° gave 0.25 g. VII. VII was also obtained from XIX at 140°. XX was recovered unchanged from refluxing MeI-MeOH after 20 h. At 110° VII was formed. XXII (0.53 g.) refluxed 13 h. with 0.05 g. Na₂CO₃ and excess MeI in alc. yielded 2,7-bis(ethoxycarbonylamino)-9-(N-methyl-p-ethoxycarbonylaminoanilino)-phenanthridine-HI, m. 250-5° (decompn.) (from Me₂COEt₂O); the base, amorphous, m. 210-20° (decompn.) (from aq. alc.). V (0.25 g.) and 0.1 g. PO₂ in 50 mL. dioxane when shaken with H gave an uptake of 160 mL. in 0.5 h. and the residue yielded the diamino chloro compd., yellow prisms, decomp. above 200° (from Me₂CO-C₆H₆), sol. in dil. HCl and pptd. unchanged by alkali. The chloride of I was inactive against Trypanosoma rhodesiense and was effective, but not curative, against T. Congolese. XIII, XXI, and IV hydrochloride were inactive against both organisms.
 IT 666236-95-9, Phenanthridine, 3,8-diamino-6-anilino-
 (and derivs.)
 RN 666236-95-9 CA
 CN Phenanthridine, 3,8-diamino-6-anilino- (5CI) (CA INDEX NAME)



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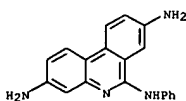
L8 ANSWER 66 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 50:13544 CA
 ORIGINAL REFERENCE NO.: 50:28411,2842a
 TITLE: Chemical constitution and antituberculous activity. III. Heterocyclic bases
 AUTHOR(S): Cymerman-Craig, J.; Rubbo, S. D.; Loder, J. W.; Pierson, Barbara J.
 CORPORATE SOURCE: Univ. Sydney, Australia
 SOURCE: British Journal of Experimental Pathology (1955), 36, 261-7
 CODEN: BJEPAS; ISSN: 0007-1021
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Pyridines, quinolines, acridines, phenanthridines, benzacridines, dibenzacridines, nicotinamides, nicotinamides, and benzimidazoles were tested for antituberculous activity, and those containing a primary NH₂ were investigated in detail. Activity is proportional to the planar surface area of the mol. and by means of this factor, combined with those described in the previous paper, a 2000-fold increase of activity was accomplished. Marked specificity of antituberculous action was present.
 IT 832-68-8, Phenanthridine, 6-amino- (antitubercular activity of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



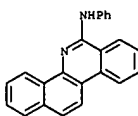
L8 ANSWER 67 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 49:54045 CA
 ORIGINAL REFERENCE NO.: 49:10438a-e
 TITLE: Properties of a small bacteriophage and the action of some compounds on it
 AUTHOR(S): Mills, R. F. N.
 CORPORATE SOURCE: Boots Pure Drug Co., Ltd., Nottingham, UK
 SOURCE: Journal of General Microbiology (1955), 12, 172-9
 CODEN: JGMIAN; ISSN: 0022-1287
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Study of the multiplication of phage S13 showed that a latent period of 20 min. existed when Escherichia coli was the host, and intracellular multiplication was only detected at the end of the latent period. Photoreactivation of phage inactivated by UV light was observed. Of 1600 chemical compds. tested for ability to inhibit phage multiplication without affecting the host cells, only the following 13 were found worthy of further study: 4,4'-di-2-imidazolin-2-ylstilbene dihydrochloride monohydrate (I), 2-hydroxy-4,4'-stilbenedicarboxamide dihydrochloride dihydrate, phenylguanidine, 1,2-bis(4'-amidino-4-biphenyloxy)ethane dihydrochloride, 1,4-bis(4'-amidino-4-biphenyloxy)butane dihydrochloride, bis(p-picolinamidophenyl) ether, bis(p-(p-methoxyphenyl)amidino)phenyl ether, 6-(p-aminoanilino)phenanthridine, 3,8-diamino-6-anilino-phenanthridine, 3,8-di-2-imidazolin-2-yl-6-phenylphenanthridine trihydrochloride dihydrate
 (II), 3,8-diamino-5-methyl-6-p-tolylphenanthridinium bromide, 3,8-diamino-5,6-dimethylphenanthridinium bromide (III), and 2,4,5,6-tetraaminopyrimidine sulfate monohydrate. Further study of the activity of I showed that multiplication early and late in the latent period was inhibited. When the 13 compds. were tested for inhibition of multiplication of T1 E. coli phage only I, II, and III inhibited phage multiplication. I had previously been reported to inhibit multiplication of Pseudomonas aeruginosa phage (Dickinson and Codd, C.A. 46, 10295d).
 IT 666236-95-9, Phenanthridine, 3,8-diamino-6-anilino- (effect of bacteriophages)
 RN 666236-95-9 CA
 CN Phenanthridine, 3,8-diamino-6-anilino- (5CI) (CA INDEX NAME)



L8 ANSWER 68 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 49:46284 CA
 ORIGINAL REFERENCE NO.: 49:8969b-f
 TITLE: Polynuclear heterocyclic systems. VIII. Synthetic applications of the Schmidt reaction
 AUTHOR(S): Badger, G. M.; Seidler, J. H.
 CORPORATE SOURCE: Univ. Adelaide
 SOURCE: Journal of the Chemical Society, Abstracts (1954) 2329-33
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 49:46284
 AB cf. C.A. 48, 11413e. The Schmidt reaction with 5,6-chrysenequinone gives 2-(o-carbamoylphenyl)-1-naphthoic acid (I), while the Beckmann rearrangement of chrysenequinone monoxime forms I and the isomeric 2-(o-carboxyphenyl)-1-naphthamide (II). By treatment with NaN₃ in H₂SO₄ I and II were converted into 1,2-benzophenanthridone (III) and 7,8-benzophenanthridone (IV), resp. III (2 g.) was refluxed 4 hours with 18 cc. POCl₃ and 0.6 cc. PhNHMe₂, excess POCl₃ removed, residue poured into cold H₂O and extracted with C₆H₆, evaporation of the C₆H₆ and recrystn. from EtOH gave 90% 9-chloro-1,2-benzophenanthridine (V), m. 156.5°, sublimes at 120° at 5 × 10⁻⁵ mm. V and PhNH₂ gave 2-anilino-1,2-benzophenanthridine, m. 152°. 1,2-Benzophenanthridine (VI) was obtained by (a) hydrogenation of V in alc. KOH over Raney Ni (86% yield); (b) treatment of III with LiAlH₄ in dioxane (giving presumably the CH₂ analog, m. 213°), followed by dehydrogenation with Pt on asbestos in cymene (95% yield); or (c) reduction of V with LiAlH₄ in dioxane (100% yield). IV (1 g.) and POCl₃ gave, similarly to the above, 0.83 g. 9-chloro-7,8-benzophenanthridine (VII), m. 163°. VII with EtOH and POCl₃ or NaOEt gave 9-ethoxy-7,8-benzophenanthridine, m. 125.5°. VII was changed back to IV by refluxing in EtOH or alc. HCl, although V was unaffected by these treatments. VII with PhNH₂ gave 9-anilino-7,8-benzophenanthridine, m. 155°. VII was converted to 7,8-benzophenanthridine by methods similar to those used for converting V to VI.
 IT 853914-25-7, Benzo[c]phenanthridine, 6-anilino- (preparation of)
 RN 853914-25-7 CA
 CN Benzo[c]phenanthridine, 6-anilino- (5CI) (CA INDEX NAME)



L8 ANSWER 69 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

ORIGINAL REFERENCE NO.: 48:1359f-1,1360a-b

TITLE: Synthesis of 1-azapyrene and phenanthrylene-4,5-methane

AUTHOR(S): Medenwald, Hans

CORPORATE SOURCE: Tech. Hochschule, Karlsruhe, Germany

SOURCE: Chemische Berichte (1953), 86, 287-93

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Heating 25 g. phenanthrene-4-aldehyde-5-carboxylic acid (I) in 250 cc. 2N NaOH and 200 cc. H₂O with a saturated aqueous solution of 8.5 g.H₂NOH.HCl 1 hr. at

90-100° gives 26.5 g. 4-oxime which, treated with 200 cc. SOCl₂, gives 70% 4-cyanophenanthrene-5-carboxylic acid chloride (II), stout crystals, m. 220°. Slowly heating 26.5 g. II in 110 cc. H₂O and 250 cc. concentrated H₂SO₄, finally 1.5 hrs. at 125-40° under reflux, and diluting with H₂O give 21 g. phenanthrene-4,5-dicarboxylic acid (III), m. 260° with loss of H₂O. Heating 3-4 g. III at 260-90° gives 70-5% phenanthrene-4,5-dicarboxylic anhydride (IV), needles, m. 260°. Adding 15 cc. concentrated NH₄OH to 3.4 g. IV in 100 cc. boiling dioxane gives 87% NH₄ salt of phenanthrene-4-carboxylic acid-5-carbamide (V) which, decomposed with 2N HCl, gives V, m. 195-235°, probably with the formation of the 4,5-imide. Heating 1.55 g. V in 40 cc. 2N NaOH with 17 cc. NaOBr solution (prepared from 3.5 g. NaOH and 4 g. Br in 50

cc. H₂O), adding 60 cc. H₂O, heating the mixture 0.75 hr. on a water bath,and saturating it with SO₂ give 50% 2-oxo-1,2-dihydro-1-azapyrene[5(4H)-thebenidinone] (VI), m. 340°. Adding 1.8 g. Na₂S to 6 g. Iin 26 cc. concentrated H₂SO₄ overlaid with 100 cc. CHCl₃, dilutingthe mixture with ice to 400 cc., distilling off the CHCl₃, and refluxing the residue

15 min. give 25% VI. Heating the Ba salt from 5 g. III at 380-415°/12 mm. gives 47% phenanthrylene-4,5-ketone (4H-cyclopenta[def]phenanthren-4-one) (VII), long yellow needles, m. 170° (oxime, light yellow needles, m. 252°). Heating 0.5 g. VI with 5 g. Zn dust with the free flame and purifying the reaction product by sublimation give 6% 1-azapyrene, m. 157-9°. Heating 6.5 g. II with 3 g. Na₂S in 125 g. moist dioxane 3 hrs. at 90-100°, evaporating the mixture with 10 cc. concentrated HCl on a water bath, and making the residue in 250 cc. H₂O

alkaline with 2N NaOH give 75% 2-imino-1,2-dihydro-1-azapyrene (VIII), needles, m. 237° (Ac derivative, prepared by boiling with Ac₂O, long needles, m. 238°). VIII in dioxane or AcOH fluoresces blue-violet. Refluxing 220 mg. VII with 0.3 g. N₂H₄.H₂O, 0.2 g. KOH, and 4 cc. (CH₂OH)₂ 10-15 hrs. gives 60% phenanthrylene-4,5-methane (4H-cyclopenta[def]phenanthrene), leaflets, m. 114-15°. Refluxing 3.2 g. II in 100 cc. dioxane with 10 cc. concentrated HCl 1.5 hrs. gives 70% phenanthrene-4,5-dicarboximide (IX), m. 240°, which is also obtained in 90% yield when equal amts. of urea and IV are heated at 180°. Treating IX in dioxane with CH₂N₂ in ether at 25-30° gives the N-Me derivative, needles, m. 176°. The infrared absorption curves of VI and IX are given.

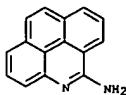
L8 ANSWER 69 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

IT 857750-48-2, Thebenidine, 4,5-dihydro-5-imino-

(preparation of)

RN 857750-48-2 CA

CN Thebenidine, 4,5-dihydro-5-imino- (SCI) (CA INDEX NAME)



L8 ANSWER 70 OF 77 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 47:57463 CA

ORIGINAL REFERENCE NO.: 47:9724b-f

TITLE: Lipoid-water partition coefficients of some aromatic bases

AUTHOR(S): Cymerman, J.; Diamantis, A. A.

CORPORATE SOURCE: Univ. Sydney, Australia

SOURCE: Journal of the Chemical Society, Abstracts (1953) 1619-21

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Apparent partition const., k, between liquid paraffin and aqueous

phosphate buffer (pH 7.2) were determined at 20° by spectrophotometric examination

of the aqueous phase for a number of aromatic bases exhibiting

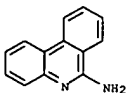
tuberculostatic activity. Values of k (given as B₀/[B₀ + B_H⁺], where B₀ and B_H are concns. of undissocd. base) are listed for the following hydrochlorides: p-2-pyridylaniline (2HCl), m. 310-13° decompose, 0.47; o-aminophenol, <1; p-aminophenol, <1; p-piperidinoaniline (2HCl), 1.28; p-toluidine, 2.00; p-chloroaniline, 3.14; 2-naphthylamine, 9.5; 1-naphthylamine, 9.7; 2-aminofluorene (m.p. 321-2°, decompose, from MeOH), 57; 2-aminochrysene (m.p. 274-5°, decompose, from MeOH), insol. in H₂O; 9-aminophenanthrene (m.p. 278-80°), 72; 4-aminoquinoline (m. 308°, from MeOH, anhydrous after drying at 120°), 0.02; 5-aminoacridine, 0.15; 5-amino-1-methylacridine 0.19; 5-amino-1,2-benzacridine (m.p. 380°, decompose, from MeOH), 4.90; 9-aminophenanthridine (m.p. 309°), 3.10; 9-amino-3-methylphenanthridine (m.p. 349-50°), 8.30; 9-amino-1,3-dimethylphenanthridine (m.p. 372°, decompose), 47.0; N'-p-biphenyl-N,N-diethylethylenediamine (2HCl), 44.7; N-p-biphenyl-2-morpholinoethylamine (2HCl), 74.9; 4-(2-diethylaminoethoxy)biphenyl, 104; 4-benzylamino-4'-dimethylaminobiphenyl (2HCl), 45.0. Other compds. for which k is given are: N'-4-bi-phenyl-N,N-diethyl-N,N',N'-trimethylethylenediammonium

diiodide, 0.065; N-p-biphenyl-N-methyl-2-morpholinoethylamine dimethiodide, 0.16; 4-(2-diethylaminoethoxy)biphenyl methiodide, 0.12; and p-biphenyl-yltrimethylammonium iodide, 0.04. UV absorption maxima are listed for all the salts except for 2-aminochrysene-HCl.

IT 62764-43-6, Phenanthridine, 6-amino-, hydrochloride (partition between paraffin oils and phosphate buffer)

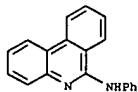
RN 62764-43-6 CA

CN 6-Phenanthridinamine, monohydrochloride (9CI) (CA INDEX NAME)

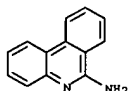


• HCl

L8 ANSWER 71 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 47:51952 CA
 ORIGINAL REFERENCE NO.: 47:8829b-c
 TITLE: The antiviral action of phenanthridinium compounds
 AUTHOR(S): Dickinson, Lois; Chantrell, B. H.; Inkley, G. W.;
 Thompson, Mildred J.
 CORPORATE SOURCE: Boots Pure Drug Co., Ltd., Nottingham, UK
 SOURCE: British Journal of Pharmacology and Chemotherapy (1953), 8, 139-42
 CODEN: BJPCAL; ISSN: 0366-0826
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Twenty-three phenanthridines and diazapyrenes were tested against influenza A virus in eggs, against Pb phage of *Pseudomonas aeruginosa* and against a range of gram-pos. and gram-neg. bacteria. Many compds. possessed marked antiphage action, up to 1000 times that on the bacterial host. Several compds., active against phage, possessed slight anti-influenza activity in eggs but the most promising compds. were inactive in mice. Seven of 9 compds. had a suppressive action against Rous sarcoma virus in chicks but only at a toxic dose.
 IT 846-62-8, Phenanthridine, 6-anilino- (antiviral action of)
 RN 846-62-8 CA
 CN 6-Phenanthridinamine, N-phenyl- (9CI) (CA INDEX NAME)



L8 ANSWER 72 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

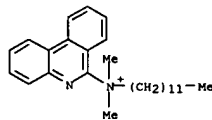


L8 ANSWER 72 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 47:51570 CA
 ORIGINAL REFERENCE NO.: 47:8750h-1,8751a-b
 TITLE: New syntheses of heterocyclic compounds. XVIII. 2,10-Diazaphenanthrenes by application of the Stieglitz rearrangement
 AUTHOR(S): Berg, S. S.; Petrov, V.
 CORPORATE SOURCE: May & Baker, Ltd., Dagenham, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1952) 3713-16
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C.A. 47, 6943e. 6-Phenylphenanthridine (C.A. numbering) (2.2 g.) and KNH2 (from 0.5 g. K) in 10 ml. liquid NH3, 48 hrs. at room temperature (sealed tube), give 600 mg. 6-aminophenanthridine, m. 188-90°. 1,3-Dimethyl-2-azafluoren-9-one (1,3-dimethyl-9H-indeno[2,1-c]pyridin-9-one) (58 g.), added (30 min.) to PhMgBr (87 g. PhBr) in 150 ml. ether, the mixture refluxed 1 hr., the cooled product diluted with 100 ml. ether, the Mg complex decomposed by refluxing 10 min. with 5 l. 2N H2SO4, and the base extracted with ether, gives 52% 1,3-dimethyl-9-phenyl-2-azafluoren-9-one (I), m. 183-4°. I (15 g.), 15 g. PC15, and 100 ml. PhMe, carefully mixed and refluxed 30 min., give 14 g. 9-chloro-1,3-dimethyl-9-phenyl-2-azafluorene (II), m. 114-16°. II (10 g.) and KNH2 (1.3 g. K) in 25 ml. liquid NH3 (3 days at room temperature) give 2.1 g. of the 9-NH2 compound (III), pale brown, m. 116-20° (picrolonate, yellow, m. above 280°). III (2.9 g.) in 75 ml. EtOH containing 700 mg. dry HCl, treated (1 hr.) at 0-5° with 20 ml. freshly prepared N KOCl, gives the 9-chloroamino compound (IV), pale yellow, m. 125-8°. IV (2 g.) in 20 ml. anhydrous C5H5N, treated with 2 g. anhydrous MeONa and kept overnight, gives 400 mg. (20%) 1,3-dimethyl-9-phenyl-2,10-diazaphenanthrene (2,4-dimethyl-6-chloro-3,5-phenanthroline) (V), m. 129-31°; with KNH2 in liquid NH3 2 g. V yields 450 mg. 9-amino analog (VI), pale brown, m. 187-9°. III (3 g.), 1.6 g. KNO3, and KNH2 (2 g. K) in 20 ml. liquid NH3 containing 50 mg. Fe(NO3)3, 5 days at room temperature, give 300 mg. of the picrate of VI. This synthesis of VI avoids the danger involved in the use of HN3 (cf. P., C.A. 40, 4379.9).
 IT 832-68-8, Phenanthridine, 6-amino- (preparation of)
 RN 832-68-8 CA
 CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)

L8 ANSWER 73 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 46:14706 CA
 ORIGINAL REFERENCE NO.: 46:2583b-c
 TITLE: Heterocyclic quaternary ammonium compounds
 INVENTOR(S): Sprague, James M.
 PATENT ASSIGNEE(S): Sharp & Dohme, Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2567912		19510911	US	

AB Quaternary ammonium compds. from Me2 (C12H25)N and RCH2X, where R is a 2-benzimidazolyl, 1-methyl-2-benzimidazolyl, or 6-phenanthridyl group and X is a halogen, are potent antibacterial agents. Dimethyldodecyl(2-benzimidazolylmethyl)ammonium chloride (I) m. 102.5-4°; 1-methyl-2-benzimidazolylmethyl analog m. 122-3°; (6-phenanthridylmethyl) analog m. 77-9°; ammonium hydroxide analog of I m. 120-1°. Other anion salts are mentioned without data.
 IT 857168-43-5, Ammonium, dodecylmethyl-6-phenanthridinyl-, chloride (preparation of)
 RN 857168-43-5 CA
 CN Ammonium, dodecylmethyl-6-phenanthridinyl-, chloride (5CI) (CA INDEX NAME)

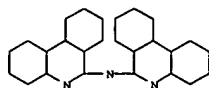


• Cl-

L8 ANSWER 74 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 45:52921 CA
 ORIGINAL REFERENCE NO.: 45:9061a-h
 TITLE: New syntheses of heterocyclic compounds. XII. The condensation of ethyl β -aminocrotonate with some cyclic amidines
 AUTHOR(S): Antaki, H.; Petrow, V.
 CORPORATE SOURCE: Univ. London
 SOURCE: Journal of the Chemical Society, Abstracts (1951) 551-5
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C.A. 44, 25311. MeC(NH₂); CHCO₂Et (I) and 9.4 g. 2-aminopyrimidine (II), heated 6-8 hrs. at 160-80° and 1 hr. at 200-20°, give 4,4a-dihydro-4-keto-2-methyl-1,4a-diazanaphthalene (III) (C.A. numbering), m. 124-5° (hydrate, m. 104-5°; picrate, yellow, m. 184°); this was considered the 4-Me derivative of Crippa and Scevola (C.A. 32, 166.6). I (5 g.), 6 g. 2-bromopyrimidine, 5 g. anhydrous K₂CO₃, and 100-200 mg. Cu bronze, heated 5-6 hrs. at 180-200°, also give III. II (9.4 g.) and 26 g. AcCH₂-CO₂Et, heated 4 hrs. at 100°, give 2-acetoacetamidopyrimidine, m. 112-13°; concentrated H₂SO₄ (24 hrs. at room temperature) gives III. I (8.5 g.) and 7 g. 2-amino-4-methylpyridine, 8 hrs. at 180-200°, give 1,4-dihydro-4-keto-2,7-dimethyl-1,4a-diazanaphthalene, m. 137° (picrate, yellow, m. 198°). 4,4a-Dihydro-4-keto-2,8-dimethyl-1,4a-diazanaphthalene, m. 130° (picrate, yellow, m. 190° (decomposition)). I (12 g.) and 10 g. 2-amino-6-methylpyridine, heated 7-8 hrs. at 190° and 2 hrs. at 210-20°, gives 1,3-bis(6-methyl-2-pyridyl)urea, m. 194° (picrate, yellow, m. 190° (decomposition)). 2-Aminoquinoline (5 g.) and 5 g. I, heated 6 hrs. at 180-200°, give 1,3-di-2-quinolylurea, m. 286°. 2-Chloroquinoline (5 g.), 4 g. I, 5 g. anhydrous K₂CO₃, and a trace of Cu bronze, heated 3 hrs. at 190° and 1 hr. at 200-20°, give 4,4a-dihydro-4-keto-2-methyl-1,4a-diazaphenanthrene, pale yellow, m. 131° (picrate, yellow, m. 207°). 6-Aminophenanthridine (C.A. numbering) gives 6,6'-diphenanthridylamine (7), yellow, m. above 310°. 2-Aminothiazole and I give 3a,4-dihydro-4-keto-6-methyl-3a,7-diazathianaphthene, pale yellow, m. 130°; it does not form a picrate but yields a H₂O-soluble HCl salt and sulfate; methiodide, m. 304° (decomposition); nitrate, pale yellow, m. 148° (decomposition); x-NO₂ derivative, yellow brown, m. 165°. 2-Amino-4-methylthiazole and I give 3a,4-dihydro-4-keto-3,6-dimethyl-3a,7-diazathianaphthene, pale yellow, m. 136°. 2-Aminobenzothiazole and I yield 4,4a-dihydro-4-keto-2-methyl-1,4a-diaza-9-thiafluorene, m. 199°; 7-acetamido derivative, m. 290° [the 7-NH₂ derivative yields a, di-HCl salt, with 1 mol. H₂O, yellow brown, m. above 266° (decomposition)]; 7-carbomethoxy derivative, m. 204-6°; 7-Cl derivative, pale yellow, m. 220°; 7-EtO derivative, m. 198°. 2-Aminonaphtho(2',1':4'5')thiazole and I give 4,4a-dihydro-4-keto-2-methyl-7,8-benzo-1,4a-diaza-9-thiafluorene, m. 207°, and 2-aminobenzoxazole (IV) yields 4,4a-dihydro-4-keto-2-methyl-1,4a-diaza-9-oxafluorene, m. 146°. IV

L8 ANSWER 75 OF 77 CA COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 43:6478 CA
 ORIGINAL REFERENCE NO.: 43:1417e-1,1418a-1,1419a-1,1420a-1,1421a
 TITLE: Some syntheses in the benzquinoline, benzacridine, and phenanthridine series
 AUTHOR(S): Albert, Adrien; Brown, D. J.; Dueswell, Heinz
 SOURCE: Journal of the Chemical Society, Abstracts (1948) 1284-95
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 43:6478
 GI For diagram(s), see printed CA Issue.
 AB The following compds. were prepared to demonstrate the relation between antibacterial activity and the extent of cationic ionization at pH 7; however, no such data are given in the present paper. In general, the
 NH₂ compds. were prepared by heating 2 g. of the Cl compound and 6-10 g.
 PHOH or p-MeC₆H₄OH 4 h. at 180° while passing NH₃ through at the rate of 2 bubbles/s.; the product is made alkaline to orange-II paper with NaOH and the precipitate repeatedly extracted with dilute AcOH; the exts., adjusted to pH 6, filtered, and made strongly alkaline, give the desired amide.
 4-Chloro-5,6-benzquinoline gives 75% of the 4-NH₂ derivative, m. 149-50°; 4-amino-7,8-benzquinoline, m. 173-4°, 75%.
 4-Hydroxy-2-methyl-5,6-benzquinoline (2 g.) and 6 mL. POCl₃, refluxed 1 h. and the sticky residue stirred with ice and NH₄OH, give 85% of the
 4-Cl compound (I), m. 99-100°; with p-MeC₆H₄OH, I yields 95% of the 4-p-tolylxy compound, m. 137°. I (5 g.), 20 g. Ph₂O, and 0.5 g. anhydrous CuSO₄ at 200°, treated 4 h. with NH₃, give 90% 4-amino-2-methyl-5,6-benzquinoline, m. 164° (corrected).
 3,2-H₂NC10H₆CO₂Et (35 g.) and 70 mL. Ac₂O, heated 10 min. at 90°, give 36 g. of the Ac derivative (II), m. 123-4°; 25 g. II and 25 mL. POCl₃, heated about 0.5 h. at 75° and during 90 min. to 125°, the product slowly stirred into 100 mL. H₂O, the mixture heated 5 h. in a boiling water bath, the dried solid extracted with 250 mL. EtOH, the insol. portion extracted with N Na₂CO₃ and H₂O, and the acid portion purified through the Na salt, give 55%
 N-(2-carboxy-3-naphthyl)-4-hydroxy-2-methyl-6,7-benzquinoline-3-carboxamide (III), pale yellow, amorphous, with 0.5 mol. H₂O, soluble in C₅H₅N with salt formation and in (CH₃OH)₂ with decarboxylation. The EtOH filtrate yields a slimy orange acid substance [m. about 190° (decomposition)] which, on acid hydrolysis at 210°, yields only 3,2-H₂NC10H₆CO₂H (IV) and AcOH; this is apparently an anhydride of IV. Crude III, heated 3 h. with 75 mL. H₂SO₄ and 75 mL. H₂O at 210°, gives 60% 4-hydroxy-2-methyl-6,7-benzquinoline (V), buff., m. 296-8°; the solns. in H₂O, EtOH, and C₅H₅N are pale yellow with intense violet fluorescence; the acid and alkaline solns. are yellow with a green fluorescence. The crude chloride from V yields 4-amino-2-methyl-6,7-benzquinoline, pale yellow, m. 180°; the EtOH or Me₂CO solution is yellow with intense blue fluorescence. 4-Amino-2-methyl-7,8-benzquinoline, m. 149-50°, 70%.
 3-Nitro-4-hydroxyquinoline (3.45 g.) and 20 mL. POCl₃, refluxed 2 h.,

L8 ANSWER 74 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 and Et 2-ketocyclohexanecarboxylate (V) (1 hr. at 180-200°) yield 4,4a-dihydro-4-keto-2,3-cyclohexeno-1,4a-diazo-9-oxafluorene, m. 198°. 2-Aminobenzimidazole (VI) and IV or AcCH₂CO₂Et give 4,4a-dihydro-4-keto-2-methyl-1,4a-triazafluorene (VII), m. 294° (decompn.) (9-Ac deriv., m. 168°). VI and AcCH₂CO₂Et (heated at 130-40°) give the 3-Et deriv. of VII, m. 284° (decompn.); 3-Pr analog, m. 253°; 3-iso-Pr analog, m. 294°. VI and V, heated at 100° until the mixt. liquifies and then at 150-60° until it solidifies, give 4,4a-dihydro-4-keto-2,3-cyclohexeno-1,4a,9-triazafluorene, m. 296° (methiodide, decomp. about 228°). VI and Et cyclopentanecarboxylate give 4,4a-dihydro-4-keto-2,3-cyclopenteno-1,4a,9-triazafluorene, m. 304°. VI (1.3 g.) and 0.83 g. MeC(NH₂); CHCN, heated at 180°, give 4,4a-dihydro-4-imino-2-methyl-1,4a,9-triazafluorene, m. above 300°; the 2-Ph analog, yellow, m. above 300°.
 IT 95953-05-2, Phenanthridine, 6,6'-iminodi-
 (preparation of)
 RN 95953-05-2 CA
 CN Phenanthridine, 6,6'-iminodi- (7CI) (CA INDEX NAME)

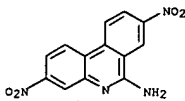


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L8 ANSWER 75 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 4-chloro-3-nitroquinoline, cream, m. 119-20°; this yields 90% 3-nitro-4-aminoquinoline, bright yellow, m. 261-2°. 3,2-H₂NC10H₆CO₂H (9.17 g.) and 275 mL. N HCl, treated at 60° with NaO₂N:CHCH₃NO₂ (from 6.03 g. MeNO₂), gives 85% 3-(2-nitroethylideneamino)-2-naphthoic acid, yellow, m. 213° (decompn.); with Ac₂O and AcONa this yields 50% 3-nitro-4-hydroxy-6,7-benzquinoline, m. above 300° (decompn.); POCl₃ gives 90% of the 4-Cl compd., orange, m. 237° (decompn.); 3-nitro-4-amino-6,7-benzquinoline (VI), orange, m. 282-3°, sol. in 700 parts EtOH at 0° and in 800 parts Me₂CO at 20°; the HCl salt is less sol. than 1 part in 5000 parts cold H₂O. VI (6.4 g.), 23.3 g. SnCl₂, 45 mL. concd. HCl, 15 mL. H₂O, and 100 mL. EtOH, refluxed 2 h., give 90% 3,4-diamino-6,7-benzquinoline, m. 212° (decompn.); it is readily oxidized in the air and was analyzed as the di-HCl salt (VII), with 2 mols. H₂O, bright yellow, m. about 310° (decompn.), very sol. in H₂O to an orange soln. with intense green fluorescence; phenanthrenequinone gives an azine, m. about 370°, which forms an intense green soln. in H₂SO₄. VII (0.56 g.) in 5 mL. H₂O, stirred at -5° with 5 mL. N HCl at -5° and then treated (5 min.) with 0.15 g. NaNO₂ in 5 mL. H₂O, gives 80% 3,4-triazolo-6,7-benzquinoline, cream, m. about 290° (decompn.); it is sol. in about 300 parts boiling EtOH; the yellow dil. soln. has a green fluorescence; the H₂SO₄ soln. is blood-red. 1,2-ClC10H₆NH₂ and AcCH₂CO₂Et, kept over H₂SO₄ 5 days, give 90% of Et β -(1-chloro-2-naphthylamino)crotonate, which, slowly added to paraform at 270° and heated for 15 min., gives 55% 8-chloro-4-hydroxy-2-methyl-6,7-benzquinoline, m. above 350°; the crude Cl deriv. (m. 159-61°) yields 65% 8-chloro-4-amino-2-methyl-6,7-benzquinoline, brownish yellow, m. 179-80°. 4-Quinolol, on nitration and redn., gives 6-amino-4-quinolol, m. 242° (decompn.); this was transformed to 1-hydroxy-p-phenanthroline by the method of Kermack and Weatherhead (C.A. 34, 7911.5); through the Cl deriv. this yields 85% 1-amino-p-phenanthroline, m. 204°. 3,2-H₂NC10H₆CO₂H (8 g.) and 8 g. cyclohexanone, slowly heated (0.5 h.) to 210°, heated 1.5 h. at 210-20°, and the product extd. with 60 mL. C₆H₆, give 50% 9-hydroxy-5,6,7,8-tetrahydro-2,3-benzacridine (C.A. numbering for acridine nucleus), yellow, m. 315°; POCl₃ gives 85% of the 9-Cl compd., cream, m. 141-2°, and this yields 75% of the 9-NH₂ compd., orange-yellow, m. 236-8°, sol. in 55 parts boiling and 400 parts ice-cold PhMe, shows an intense blue fluorescence in EtOH, and its HCl salt (VIII) dissolves in 500 parts cold H₂O with pale yellow color and blue fluorescence. A 0.2% soln. of VIII, exposed to direct sunlight 2 days, gives 95% of the polymer, (C₁₇H₁₆N₂)_n, m. 265°; the polymn. is not reversed by irradiation with light of 3650 Å. 9-Chloro-3,4-benzacridine (11 g.) in 54 g. PhOH at 70°, treated with 6 g. (NH₄)₂CO₃ (5 min.), the mixt. heated 0.5 h. at 120°, the melt poured into NaOH, the base extd. with 300 mL. N AcOH, the pH adjusted to about 6, and the filtrate made alk., gives 90% 9-amino-3,4-benzacridine, yellow, m. 196-7°; the pale yellow EtOH soln. has an intense violet fluorescence (von Braun, C.A. 21, 1122, ascribed this structure to a compd. m. 94-8°); the pale yellow HCl salt is sol. in 150 parts cold H₂O (the faint green fluorescence becomes intense violet on diln.). Details are given of the reaction of 3-HOClO₆CO₂H and PhNH₂ (10 h. at 120°) which yields 52% 3,2-HOClO₆CONHPh, 16% 3,2-PhNHClO₆CONHPh, and 28% 3,2-PhNHClO₆CO₂H; the last with POCl₃ gives 97% 9-chloro-2,3-benzacridine which yields 75% of the 9-NH₂ compd. (IX), scarlet, m. 231-2°, sol. in 17 parts EtOH (orange fluorescence) (prepd. in absence of daylight but not affected by light from a 100-w.

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incandescent lamp): Ac deriv., with 0.25 mol. H₂O, m. about 230°
(decompn.): the orange EtOH soln. has a slight green fluorescence: it is
sol. in N NaOH (scarlet) and in 2 N AcOH (purple). IX (0.244 g.) in 1
mL.
HCl and 200 mL. H₂O, boiled 5 min. in the dark and exposed to light (8
h.), gives the polymer (C₁₇H₁₂N₂.HCl.0.75-H₂O)_n, which, stirred 1 day
with
N NaOH, gives the free base, ivory, m. 310°. 9-Chloro-1,2-
benzaziridine yields 80% of the 9-NH₂ compd., golden, m. 236-7°; the
pale yellow EtOH soln. has a green fluorescence that becomes intense blue
on diln.; the cream HCl salt dissolves in 400 parts cold H₂O (violet
fluorescence on diln.). 5,1-OZNC10H₆NH₂ (4 g.), 8 g. o-
ClC₆H₄CO₂K, 0.1 g. Cu, 1.5 g. anhyd. K₂CO₃, and 40 mL. cyclohexanol,
heated 7 h. at 160-70°, the steam-distd. soln. adjusted to 300 mL.,
30 g. K₂CO₃ added, and the K salt in 40 mL. boiling H₂O acidified with
AcOH, give 21% 2-(5-nitro-1-naphthylamino)benzoic acid, light brown, m.
239°; this yields 95% 9-chloro-4'-nitro-3,4-benzaziridine which
gives 85% 4'-nitro-9-amino-3,4-benzaziridine (X), red, m. 250-2°
(decompn.), sol. in about 120 parts cold Me₂CO and 500 parts PhCl at
0°; hydrogenation of 1 g. X in 150 mL. Me₂CO with Raney Ni at room
temp. at atm. pressure gives 85% 4',9-diamino-3,4-benzaziridine,
orange-yellow, m. 225-6°, sol. in about 1000 parts PhCl at
0°; it is stable to boiling N NaOH; the mono-HCl salt is orange and
the di-HCl salt is pale yellow. The general method for the prep. of the
2-aminoquinoline analogs was to heat 3 g. of the Cl compd., 15 g.
ZnCl₂.2NH₃, and 3 g. NH₄Cl in an open tube contained in a sealed steel
tube 6 h. at 220-40°; the product in HCl was pptd. with NH₄OH to
remove the Zn, extd. with N AcOH, the filtrate adjusted to pH 5 to ppt.
unchanged Cl compd., and the base liberated with NaOH.
N-2-Naphthylacetamide (XI) m. 102° (from C₆H₆) or 92°
(from H₂O); stirred 15 min. with 9 parts concd. HCl, it gives a quant.
yield of 2-hydroxy-4-methyl-5,6-benzaziridine which with POCl₃ gives 95%
of the 2-Cl compd.; this yields 60% of 2-amino-4-methyl-5,6-
benzaziridine, m. 224-5°. AcCH₂CO₂Et (18 mL.) and 0.025 g.
Cu(OAc)₂ at 160°, treated with 5 g. 1-ClOH₂NH₂ and the mixt. heated
15 min. at 160°, give 70% of the 1-isomer of XI, m. 115-17°
(petr. ether) or 106-7° (C₆H₆); this yields 85%
2-hydroxy-4-methyl-7,8-benzaziridine and 95% of the 2-Cl compd., which
gives 40% 2-amino-4-methyl-7,8-benzaziridine, m. 133-4°.
CH₂(CO₂Et)₂ (32 g.) at 180°, treated with 7.3 g. 1-ClOH₂NH₂, the
mixt. heated 15 min. at 180°, and the crude Et N-1-
naphthylmalonamide (m. 227°) added to paraffin at 260-80°,
gives 50% 2,4-dihydroxy-7,8-benzaziridine; refluxed 2.5 h. with POCl₃,
it
yields 80% 2,4-dichloro-7,8-benzaziridine, m. 133°; this could not
be aminated. 3,8-Dinitro-6(5H)-phenanthridone (C.A. numbering) (5 g.)
and
50 mL. POCl₃, refluxed 5 h., give 97% 6-chloro-3,8-dinitrophenanthridine,
cream, m. 225°; amination gives 85% of the NH₂ compd., yellow, m.
321-2°; redn. with SnCl₂ in concd. HCl gives 70%
3,6,8-triaminophenanthridine, cream, m. 200°; the yellow EtOH soln.
has an intense green fluorescence; it diazotizes to an orange soln. which
gives a purple color with 2-ClOH₂OH. 4-Amino-2-methyl-6,7-benzaziridine
(5.01 g.) and 8.4 mL. Ac₂O, refluxed 5 min. at 155°, 8.4 mL. BzH
added, and the mixt. heated 3 h. at 155°, give 90%

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g.), 17 mL. concd. HCl, and 6.8 mL. (HCHO)₃, heated 1 h. on the water
bath, dild. with 1.5 l. 0.3 N HCl, boiled 0.5 h., the residue extd. with
3
more portions (1.5 l.) HCl, the base (pptd. with NH₄OH) boiled 15 min.
with 6 l. 0.3 N HNO₃, and immediately pptd. with NH₄OH, give 35%
6-nitro-2-methyl-7,8-benzaziridine, light yellow, m. 141-2°;
catalytic redn. in Me₂CO over Raney Ni at room temp. and atm. pressure
gives 90% 6-amino-2-methyl-7,8-benzaziridine, m. 128-9°.
1'-Nitro-2-methyl-7,8-benzaziridine (XVII), m. 153°, sol. in 50
parts cold Me₂CO, 30%; 1'-NH₂ compd., buff, m. 141-5°.
6-Nitro-2-styryl-7,8-benzaziridine, yellow, m. 142-3°, 50%
IT 855622-59-2, Phenanthridine, 6-amino-3,8-dinitro-
(preparation of)
RN 855622-59-2 CA
CN Phenanthridine, 6-amino-3,8-dinitro- (SCI) (CA INDEX NAME)



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4-acetamido-2-styryl-6,7-benzaziridine (XII), with 0.5 mol. H₂O, yellow,
m. 244°; 4.2 g. XII in 80 mL. C₅H₅N and 16 mL. H₂O, treated (1 h.)
with 5.3 g. KMnO₄ (temp. below 20°), 30 mL. H₂O added to keep the
salts in soln., and the soln. stirred with addnl. H₂O, gives 70%
4-amino-6,7-benzaziridine-2-carboxylic acid; 1 g. of the acid, added to
60 mL. paraffin at 280 ± 2° (3 min.), gives 50%
4-amino-6,7-benzaziridine, bright yellow, m. 233°; the yellow EtOH
soln. has a blue fluorescence. 4-Chloro-2-methyl-6,7-benzaziridine
(11.14
g.) in 15 mL. MeOH contg. 0.23 g. Na, refluxed 2 h., gives 90%
4-methoxy-2-methyl-6,7-benzaziridine (XIII), yellow, m. 103-5°; 1
g. XIII yields 1.3 g. of the crude styryl compd., oxidn. of which gives
4-methoxy-6,7-benzaziridine-2-carboxylic acid, yellow, m. 255°
(decompn.); demethylation by heating 3 h. at 210° with a mixt. of 3
mL. H₂SO₄ and 3 mL. H₂O and the resulting product stirred 3 min. with
paraffin at 270° give 4-hydroxy-6,7-benzaziridine, cream, m.
272-3°; the C₅H₅N soln. has a violet fluorescence; the solns. in
HCl and N NaOH are yellow with green fluorescence. 4-Chloro-3-nitro-6,7-
benzaziridine (3 g.) in 600 mL. CHCl₃, treated with 2 g.
p-MeC₆H₄SO₂NH₂
in 90 mL. CHCl₃ and, after 24 h., the pptd. hydrazide (decomp. about
170°) heated 1.5 h. with 450 mL. 0.5 N NaOH, gives 60%
3-nitro-6,7-benzaziridine (XIV), orange, m. 206°; redn. as above
gives 85% 3-amino-6,7-benzaziridine, yellow-brown, m. 240-1°; it
is sol. in about 30 parts boiling EtOH, the soln. having an intense green
fluorescence on diln. 6-Bromophenanthridine (1 g.) in 30 mL. EtOH and
about 3 g. Raney Ni, added to 0.5 g. KOH in 10 mL. EtOH and shaken with H
at room temp./atm. pressure, gives 95% phenanthridine (23 mL. of the EtOH
could be replaced by 8 mL. C₅H₅N previously refluxed 4 h. with Raney Ni).
6(5H)-Phenanthridone (2 g.) in 150 mL. EtOH contg. 0.9 g. NaOH and 50 mL.
H₂O at 85°, treated (1.5 h., CO₂ atm.) with 200 g. Na-Hg and the
mixt. heated 1.5 h. at 100°, gives 1 g. of a hexahydro deriv., m.
176-8°. 7-Nitro-3,4-benzaziridine-9(10H)-one (2.9 g.) in 150 mL.
EtOH contg. 0.9 g. NaOH and 150 mL. H₂O at 85°, treated (2 h., CO₂
atm.) with 200 g. Na-Hg, the mixt. heated an addnl. 2 h., the EtOH
removed, the residue extd. with 200 mL. boiling 1.5 N HCl, air blown
through the ext. at 95° (4 h.), and the soln. filtered into 150 mL.
2.5 N NaOH, give 50% 7-amino-3,4-benzaziridine, light brown, m.
165°, violet fluorescence in petr. ether and green in EtOH; the red
mono-HCl salt gives an aq. soln. with a green fluorescence; the di-HCl
salt is yellow. 3,2-H₂NC10H₆CO₂H (9 g.), 15 g. p-BrC₆H₄NO₂, 7.5 g.
K₂CO₃,
0.3 g. Cu, and 45 mL. PhNO₂, heated 1.5 h. at 150°, and 2 h. at
180°, give 3-p-nitroamino-2-naphthoic acid (XV), yellow, m.
260°; POCl₃, followed by hydrolysis with HCl, gives
7-nitro-2,3-benzaziridine, with 0.5 mol. C₅H₅N, yellow-brown, does not m.
at 360°; Na-Hg yields 60% 7-amino-2,3-benzaziridine, bright red, m.
285-6°, sol. in 300 parts EtOH (intense orange fluorescence),
stable to boiling N NaOH; the HCl salt is sol. in about 20 parts H₂O
(red). The m-NO₂ isomer of XV, yellow, m. 226-7°, 15%. Distn. of
2,3-benzaziridine-9(10H)-one with Zn dust gives only 15% 2,3-benzaziridine
but Na-Hg gives 70% (cf. Schopp, Ber. 27, 2840 (1894)).
6,7-Benzaziridine
results in 15% yield on heating 1 g. of the 1',2',3',4'-tetrahydro deriv.
with 0.5 g. Pd-C in 5 mL. Ph₂O 3 h. at 270°. 4,1-OZNC10H₆NH₂ (7.9

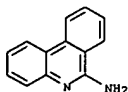
L8 ANSWER 76 OF 77 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 37:8471 CA
ORIGINAL REFERENCE NO.: 37:1432h-1,1433a-g
TITLE: A Hofmann-type rearrangement in liquid ammonia
AUTHOR(S): White, H. C.; Bergstrom, F. W.
SOURCE: Journal of Organic Chemistry (1942), 7,
497-507
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Since it has been found that 2-phenyl-4-quinolinecarboxylic acid (I) when
treated with KNH₂ and KNO₃ gives good yields of 2-phenylindole, the amide
(II) of 1, 2-(2-naphthyl)quinoline- (III), 2-(p-methoxyphenyl)quinoline-
(IV), 2-phenylbenzo [h] quinoline- (V), 2-p-xenylquinoline-4-carboxamide
(VI) and 3-phenylbenzo [f] quinoline-1-carboxamide (VII) are subjected to
the same treatment. II, m. 195-7°, is prepared in 49.7% yield by
refluxing 22.1 g. isatin, 16 g. NH₄Cl, 180 cc. concentrated NH₄OH and 20
g. PhAc
for 50 min. III, prepared from the acid chloride, m. 250.5-1°; IV m.
245-6°; V, prepared in 67% yield, m. 268-9°; VI, m.
245.5-6° is prepared from the chloride of 2-p-xenyl-4-
quinolinecarboxylic acid (VIII) which is obtained by refluxing 10 g.
p-PhC₆H₄Ac and 9 g. isatin in 100 cc. 33% KOH for 5 hrs. After cooling,
the mixture is acidified with AcOH, giving 11 g. VIII, m. 292-3°.
VII, prepared in 81% yield, m. 239-40°. When 2.48 g. II and KNH₂
from 1.17 g. K in liquid NH₃ are kept at room temperature for 23 days,
43.44
2-phenyl-4-aminoquinoline (IX), m. 163-4°, is formed. By using the
same conditions but with addition of KNO₃ or Hg, 89-98% IX is obtained in
addition to a corresponding amount of KNH₂ and KCNO. With Ba(NH₂)₂ in
lieu of
KNH₂, II gives 2-phenylquinoline as chief product. 2-Phenyl-6-methyl-4-
quinolinecarboxamide, KNH₂ and KNO₃ kept at room temperature for 4 days
give a
reddish brown tar from which 2-phenyl-4-amino-6-methylquinoline, m.
184-5°, is isolated. V, KNH₂ and KNO₃ give 54%
2-phenyl-4-amino-6-methylquinoline, m. 162.5-3°. The NHMe or NMe₂
derivative of I with KNH₂ and KNO₃ gives IX in 78.5% and 23.3% yield,
resp.
o-BzC₆H₄CONH₂, KNH₂ and KNO₃ at 20° for 6 days give 20%
o-BzC₆H₄NH₂, m. 105-7°, and 51% KNO₂. 2-p-Tolyl-4-
quinolinecarboxamide, III, IV and VI with KNH₂ and KNO₃ give only tars.
PhCH₂CONH₂ dissolves in KNH₂ and liquid NH₃ with a deep color,
probably due to the formation of PhCH₂CONH₂, and after treatment with
KNO₃
up to 74% is recovered without formation of any KNO₂. C₁₈H₁₃CONH₂ and
2-propyl-2-phenyl-4-methylpentanamide do not react with KNH₂ and KNO₃.
4-Quinolinecarboxamide, KNH₂ and KNO₃ kept for 2 days give 54%
2-amino-4-quinolinecarboxamide (X), m. 218-18.5°; picrate m.
278-80° (decomposition). Saponification of X gives the acid, m. 349-53°.
The results indicate that the reaction occurs only if the CONH₂ group is
activated by CO or CN at a favorable position in the mol. When 0.71 g.
2-phenyl-4-quinolyl isocyanate (XI), 0.4 g. KNO₃ and KNH₂ from 0.35 g. K
are allowed to react for 2 days, 77% of XI is recovered, but with 5
equivalent
KNH₂ and 1 equivalent KNO₃ for 36 hrs., 62% XI and 20% IX are obtained.
2-Phenyl-6-methyl-4-quinolyl isocyanate (XII), prepared according to John
(C. A. 25, 3427), m. 246-7° instead of 214° as reported;
picrate m. 206-7°. XII, KNH₂ and KNO₃ after 2 days at room temperature
are recovered unchanged. PhNCO (XIII) in liquid NH₃ gives 87.5%

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 PHNCONH2, m. 144-5°, while addn. of KNO2 gives (PhNH)2 CO, m. 233-4°. 1-ClOH7NCO (XIV) and KNO2 in liquid NH3 at -33° give 48% 1-ClOH7HNCONH2 (XV), m. 211-12°, and 38% (1-ClOH7HN)2CO (XVI), m. 283-5°. When to 1-ClOH7NHK from 4 g. amine in liquid NH3, 4 g. XIV is slowly added and the reaction stopped after 10 min. by addn. of NH4Cl, 55% XV and 38% XVI are formed. When 0.384 g. HCONH2, 1.1 g. KNO3 and KNO2 from 0.7 g. K are kept for 18 hrs. in a sealed tube, 176.6 cc. gas, contg. 97.5% H, is formed. 9-Amino-9-phenylfluorene, KNO2 and KNO3 give 61% 9-aminophenanthridine, m. 190-0.5°. Ph3CNH2, KNO2 and KNO3 at 80° for 14 hrs. in a steel bomb give 43% BzNH2. Apparently a Stieglitz-type rearrangement takes place with the formation of Ph2C:NPh, which is split to PhC(:NH)NHK and this is hydrolyzed to BzNH2. The mechanisms of these reactions are discussed.

IT 832-68-8, Phenanthridine, 6-amino-
 (preparation of)

RN 832-68-8 CA

CN 6-Phenanthridinamine (9CI) (CA INDEX NAME)



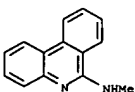
L8 ANSWER 77 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)
 though very slowly. 5,2-O2N(H2N)C6H3Ph and p-O2NC6H4COCl in C5H5N give 5-nitro-2-p-nitrobenzamidobiphenyl, buff, m. 209°; refluxing with POCl3 for 30 h. gives 3-nitro-9-p-nitrophenyl-phenanthridine, pale yellow, m. 294°; catalytic redn. gives the 3-amino-9-p-aminophenyl deriv., m. 233°; HBr salt, with 1 mol. H2O, orange plates; sulfate, cream needles; di-Ac deriv., m. 327-8° (decomp.); p-MeC6H4SO3Me in PhNO2 gives the pale orange p-toluenesulfonate, converted to 3-acetamido-9-p-acetamidophenyl-10-methylphenanthridinium chloride, pale yellow needles; the free di-NH2 chloride, with 0.5 mol. H2O, forms transparent, red prismatic needles. The following were prepd. in substantially the same way as their isomers. 4'-Nitro-2-p-nitrobenzamidobiphenyl, m. 208°; 7-nitro-9-p-nitrophenylphenanthridine, m. 327°; 7-amino-9-p-aminophenyl deriv., pale yellow, m. 212°; the red HCl salt is extremely sol. in H2O; the sulfate forms brick-red talc-like crystals; di-Ac deriv., m. 172-3°. 7-Acetamido-9-p-acetamidophenyl-10-methylphenanthridinium p-toluenesulfonate, yellow needles or transparent prisms; chloride, with 1.5 mol. H2O, yellow prisms; the free di-NH2 chloride, with 0.5 mol. H2O, ruby-red, m. 262° (decomp.). 4'-Nitro-2-benzamidobiphenyl, m. 165.5°; 7-nitro-9-phenylphenanthridine, pale yellow, m. 237°. 5,4'-Dinitro-2-benzamidobiphenyl, m. 250°; it gives a very small yield of 5,7-dinitro-9-phenylphenanthridine, yellow, m. 275-7°. Heating 9-chlorophenanthridine (VI) and 33% MeOH-MeNH2, at 180° for 5 h. gives 9-methylaminophenanthridine, m. 187°; sulfate, needles, the 2% aq. soln. of which had pH 6-6.5; Ac deriv., m. 155°; 9-dimethylamino homolog (VII), m. 61.5°; HCl salt, needles, the 2% aq. soln. of which had pH 4.5-5. VI and Me3N, followed by KI, give 9-phenanthridyltrimethylammonium iodide, m. 234° (decomp.); the 2% aq. soln. has a pH of 5.5. VII and MeI, heated at 125° for 4 h., give 9-dimethylamino-10-methylphenanthridinium iodide, yellow, m. 230° (decomp.); heating the aq. soln. gives N-methylphenanthridone. 9-phenanthridylmethyltrimethylammonium iodide, m. about 222° (decomp.), results from 9-phenanthridylmethylphenanthridine and MeNH2 at 100° for 2 h., followed by KI; C5H5N gives 9-phenanthridylmethyl-N-pyridinium chloride (VIII), decomp. about 250°; the 2% aq. soln. had a pH of 6.5°; the nitrate, sulfate and perchlorate were sparingly sol. in H2O; piperidine gives 9-phenanthridylmethylphenanthridine, pale yellow, m. 90-3°; HCl salt, with 1 mol. H2O, prisms; the 2% aq. soln. had pH 5.5. A report is given on the antiseptic action of 31 phenanthridine compds. and certain relations between constitution and action are discussed. VIII is among the most active members of the series

for Staphylococcus and B. coli in serum as well as in aq. soln.

IT 951-07-5, Phenanthridine, 6-methylamino-
 (preparation of)

RN 951-07-5 CA

CN Phenanthridine, 6-(methylamino)- (6CI, 7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 77 OF 77 CA COPYRIGHT 2005 ACS on STN
 32:33042 CA
 ORIGINAL REFERENCE NO.: 32:4588c-1,4589a-f
 TITLE: Phenanthridine series. V. The color and antiseptic properties of quaternary salts
 Morgan, Gilbert T.; Walls, Leslie P.; Browning, C. H.;
 AUTHOR(S): Gulbransen, R.; Robb, J. V. M.
 SOURCE: Journal of the Chemical Society, Abstracts (1938) 389-97
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB cf. C. A. 30, 103.5. The work reported in parts I and II (C. A. 26, 461, 5956) drew attention to the color of certain quaternary salts of the series, which also contained primary NH2 groups. Further information has been obtained by replacement of the latter by tert-NH2 groups and by the study of other series of salts. 3-Amino-9-methylphenanthridine (I) yields

a HCl salt, yellow, with 2 mols. H2O. I and MeI, heated at 150° for 6 h., give 3-dimethylamino-9-methylphenanthridine, brown, m. 146°; pure quaternary salts could not be obtained therefrom by further methylation; HCl salt, red needles. 3-Acetamido-9,10-dimethylphenanthridinium methosulfate and KI give the iodide, yellow needles; AgCl gives the chloride, pale yellow needles, with 1 mol. H2O. 9-p-Aminophenylphenanthridine (II) yields a red mono-HCl salt; II with MeI

at 150° for 8 h. gives 9-p-dimethylaminophenylphenanthridine (III), buff, m. 179-81°; HCl salt, orange-red, transparent plates. 9-p-Aminophenyl-10-methylphenanthridinium iodide (IV), ruby-red, transparent prisms. p-Acetamidophenyl-10-methylphenanthridinium chloride, pale orange prisms, with 2 mols. H2O. Heating III with p-MeC6H4SO3Me in PhNO2 at about 180° gives a dark red solution, from which a white p-toluenesulfonate seps.; this was converted into 9-phenanthridyl-p-phenyltrimethylammonium iodide, m. 179° (decomposition); the red melt solidified and then m. 235° (conversion into an isomer(?)); the red aqueous liquor after steam distillation of PhNO2 gives

9-p-dimethylaminophenyl-10-methylphenanthridinium p-toluenesulfonate, with 2 mol. H2O, m. with loss of H2O at 120°, forming a dark red glass; iodide (V), brick-red prisms, m. 238° (decomposition); chloride, hydrated ruby-red prisms, with Cu reflex. When III is methylated with Me2SO4 a diquaternary dimethosulfate is formed, characterized as the diiodide (VI), pale yellow prisms, m. 232-6° (decomposition); the same salt was obtained in high yield when a large excess of p-MeC6H4SO3Me was used; the white chloride lost MeCl slowly at 100° to yield the red monochloride. Heating IV with MeI at 180° for 7 h. gives V and VI. In this series the bases, primary and tertiary, and Ac derivs. are colorless or almost so, but monoacid salts and those with the hetero-N alone quaternary are red. The appearance of color is always associated with the possibility of tautomerism, probably due to wave-mech. resonance. In the synthesis of phenanthridine derivs. from acyl-o-xenylamines by POCl3 considerable resinification may occur, probably due to a side reaction involving elimination of the acyl group. The side reaction predominates when R in 4-R'C6H4C6H3(NHCOR)-2-R''-5 is Me, R' is NO2 and R'' is H or NO2; if R is Ph or p-O2NC6H4 the side reaction is suppressed and ring closure occurs,

L8 ANSWER 77 OF 77 CA COPYRIGHT 2005 ACS on STN (Continued)

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(FILE 'HOME' ENTERED AT 15:37:17 ON 08 SEP 2005)

FILE 'REGISTRY' ENTERED AT 15:37:36 ON 08 SEP 2005

L1 STRUCTURE UPLOADED

L2 38 S L1 SAM

L3 666 S L1 FULL

FILE 'CA' ENTERED AT 15:38:01 ON 08 SEP 2005

L4 151 S L3

L5 90 S L4 AND PY<1999

L6 12 S L5 AND (PHARM? OR DRUG?)

L7 78 S L5 NOT L6

L8 77 S L7 AND PY<1998

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 15:39:51 ON 08 SEP 2005